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ESN (EUROPEAN SCIENCE NOTES INFORMATION BULLETIN)
REPORTS ON CURRENT EUROPEAN/MIDDLE EASTERN SCIENCE(U)
OFFICE OF NAVAL RESEARCH LONDON (ENGLAND) C J FOX
APR 88 ESN-88-03

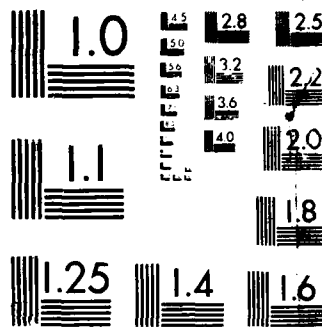
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ESN INFORMATION BULLETIN

European Science Notes Information Bulletin
Reports on Current
European/Middle Eastern Science

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DISTRIBUTION STATEMENT A

Approved for public release;
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SECURITY CLASSIFICATION OF THIS PAGE

REPORT DOCUMENTATION PAGE

1a REPORT SECURITY CLASSIFICATION UNCLASSIFIED		1b RESTRICTIVE MARKINGS	
2a SECURITY CLASSIFICATION AUTHORITY		3 DISTRIBUTION / AVAILABILITY OF REPORT Approved for public release; distribution unlimited	
2b DECLASSIFICATION / DOWNGRADING SCHEDULE			
4 PERFORMING ORGANIZATION REPORT NUMBER(S) 88-03		5 MONITORING ORGANIZATION REPORT NUMBER(S)	
6a NAME OF PERFORMING ORGANIZATION Office of Naval Research Branch Office, London		6b OFFICE SYMBOL (If applicable) ONRBRO	
6c ADDRESS (City, State, and ZIP Code) Box 39 FPO, NY 09510-0700		7a NAME OF MONITORING ORGANIZATION	
7b ADDRESS (City, State, and ZIP Code)		8a NAME OF FUNDING / SPONSORING ORGANIZATION	
8b OFFICE SYMBOL (If applicable)		9 PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER	
8c ADDRESS (City, State, and ZIP Code)		10 SOURCE OF FUNDING NUMBERS	
		PROGRAM ELEMENT NO	PROJECT NO
		TASK NO	WORK UNIT ACCESSION NO
11 TITLE (Include Security Classification) European Science Notes Information Bulletin - (UNCLASSIFIED)			
12 PERSONAL AUTHOR(S) C.J. Fox, Editor			
13a TYPE OF REPORT Multidiscipline	13b TIME COVERED FROM TO	14. DATE OF REPORT (Year, Month, Day) April 1988	15 PAGE COUNT 81
16 SUPPLEMENTARY NOTATION			
17 COSATI CODES		18 SUBJECT TERMS (Continue on reverse if necessary and identify by block number)	
FIELD	GROUP		
19 ABSTRACT (Continue on reverse if necessary and identify by block number)			
<p>The European Science Notes Information Bulletin (ESNIB) is a compilation of reports on recent developments in European science of specific interest to the US R&D community, and is issued in support of the mission of the Office of Naval Research Branch Office, London. It is not intended to be part of the scientific literature. The value of the Bulletin to Americans is to call attention to current activity in European science and technology and to identify the institutions and people responsible for these efforts. ESNIB authors are primarily ONRL staff members; other reports are prepared by or in cooperation with staff members of the USAF European Office of Aerospace Research and Development or the US Army Research, Development and Standardization Group. US scientists travelling in Europe may also be invited to submit reports.</p>			
20 DISTRIBUTION / AVAILABILITY OF ABSTRACT <input checked="" type="checkbox"/> UNCLASSIFIED UNLIMITED <input type="checkbox"/> SAME AS RPT <input type="checkbox"/> DTIC USERS		21 ABSTRACT SECURITY CLASSIFICATION UNCLASSIFIED	
22a NAME OF RESPONSIBLE INDIVIDUAL C.J. Fox		22b TELEPHONE (Include Area Code) (44-1) 409-4340	22c OFFICE SYMBOL 310

This publication is approved for official dissemination of technical and scientific information of interest to the Defense research community and the scientific community at large.

Commanding Officer CAPT Terry J. McCloskey, USN
Scientific Director James E. Andrews
Editor C.J. Fox

The Nobel Prize Ceremonies for 1987 Alan F. Clark 1

This is a personal, eye-witness account of the pageantry, ceremony, and social events attendant to the awarding in Stockholm of the Nobel prizes.

ACOUSTICS

→ Natural Mechanism of Surface-Generated Noise in the Ocean, NATO Advance Research Workshop W.A. Kuperman 3

The results of the five topics of this workshop, held in June 1987 at Lerici, Italy, are discussed. The topics are: wave and turbulence noise, distribution of bubbles and turbulence in and near a breaking wave, origins of surface-generated noise at intermediate and high frequencies, and ice noise.

BEHAVIORAL SCIENCES

Self-Concept and Adjustment - Research by Portugal's Adriano Vaz-Serra; William D. Crano 5

The current work in self-concept and adjustment by Professor Vaz-Serra and colleagues at the University of Coimbra is reviewed. This report includes discussion of the clinical inventory of self-concept and the problems-resolution inventory which Vaz-Serra developed for his studies of self-concept and coping and of the relations between self-concept and coping. These studies, with tables showing the results, are also discussed.

Forthcoming European Conferences in Psychology William D. Crano 11

Two forthcoming European Conferences in Psychology are briefly described and the vital information given.

BIOLOGICAL SCIENCES

Medicinal Chemistry Symposium, Cambridge, UK; Claire E. Zomzely-Neurath 12

Selected presentations given at this symposium, held in September 1987, are summarized. The topics include: neuropeptides; control of enzymatic processes in medicinal chemistry; antiviral agents; antibacterial, antifungal, and antiparasitic agents, and application of computing to medicinal chemistry.

Biotechnology Conference - Extremophiles: Exploration and Exploitation Claire E. Zomzely-Neurath 19

Summaries of selected papers presented at this conference, held in December 1987 in London, UK, are given. Topics include: bacteria from alkaline and saline environments, metal leaching by acidophilic bacteria, extreme bacteria and osmotic stress, thermostable enzymes for biotechnology, and halobacteria.

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Biotechnology Conference Diagnostics '87 ; Claire E. Zomzely-Neurath 25

Presentations given at this conference held in December 1987 in Cambridge, UK, are briefly summarized. The presentations covered the impact of new technologies on diagnostics, and a number of specific diagnostic systems, methods, and technologies.

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Selected papers presented at this meeting, held in Maastricht, the Netherlands, in September 1987, are summarized. The topics are: measuring electrical events; electrodeposition; and batteries, fuel cells, and materials.

The Fifth International Topical Meeting on Photoacoustic and Photothermal Phenomena ; Jane K. Rice 30

Brief summaries are given of presentations made at this conference held in Heidelberg, West Germany, in July 1987. Topics include kinetics and relaxation; biological applications, trace analysis and detection, surface and thin films, and nondestructive evaluation.

COMPUTER SCIENCES

Engineering Applications of Transputers Initiatives ; J.F. Blackburn 33

The UK government is supporting the development of engineering application of the Inmos company's transputer products. The author reviews the background for, gives a progress report on, and looks at the future of this government-sponsored initiative to realize the benefits promised by transputers.

The Edinburgh Concurrent Supercomputer Center ; J.F. Blackburn 35

This Center, staffed by Edinburgh University personnel, is being equipped with a transputer-based concurrent supercomputer. The Center's programing developments to date, which cover a wide range of applications, are discussed.

Vector and Parallel Processors in Computational Science III J.F. Blackburn 40

Fourteen of the 40 papers given at this conference held in August 1987 in Liverpool, UK, are summarized. Parallel computer architecture, programing for parallel systems, and the adaptability of a variety of applications to parallel processing were covered.

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This institute, a DFVLR laboratory located near Munich, West Germany, is primarily concerned with guidance and control of robots, surface vehicles, and dynamic systems (with special reference to aerospace vehicles). These activities are discussed.

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- Fluid Mechanics at the Netherlands' National Aerospace Laboratory** Daniel J. Collins 48

The experimental and theoretical activities of the National Aerospace Laboratory's Fluid Mechanics Division are briefly reviewed, with particular emphasis on computational fluid dynamics.

MATERIAL SCIENCES

- Fifth European Conference on Internal Friction and Ultrasonic Attenuation in Solids** R.W. Judy 51

The six invited lectures given at this conference, held in July 1987 in Antwerp, Belgium, are briefly reviewed in this report, along with summarizing comments about the contributed papers in general.

- Wear Resistant Materials in France** Louis Cartz 53

This meeting, "Surface Treatment of Wear Resistant Materials," was held in November 1987 at St. Etienne, France. Presentations on ion implantation techniques, vapor deposition, and thermal/laser treatment are reviewed.

- Engineering Ceramics at the European Research Center at Petten, the Netherlands** Louis Cartz 57

This report concerns the high-temperature materials studies, particularly on the stability of materials in severe environments, which are carried out at the European Joint Research Center at Petten. Included are studies of high-temperature corrosion problems, behavior of Si_3N_4 ceramic, corrosion in O, C/O, and S/O atmospheres, and mechanical properties.

- Refractories Meeting in Germany** Louis Cartz 59

A brief summary of this meeting held in October 1987 at Aachen, West Germany, is given. Most of the talks were concerned with practical systems.

PHYSICS

- Quantum Optics, Optoelectronics, and Laser Spectroscopy at the General Meetings of the European Physical Society** Paul Roman 61

Following a brief overall review of the 7th General Conference of the European Physical Society (EPS-7) in Helsinki, August 1987, selected talks in the areas of quantum optics, electro-optics, optronics, and laser spectroscopy are described in some detail.

- Advanced X-ray Research at Garching** Paul Roman 64

A research group at the Max Planck Institute for Quantum-Optics concentrates its work on producing soft x-ray black body Planck radiation in tiny cavities, excited by powerful laser radiation. Brightness-temperatures around 2×10^6 K have been achieved; the radiation spectrum peaked between 20 and 50 Å. Other work of the group involves spectrum analysis of x-ray radiation emitted by laser plasmas.

- 12th International Conference of Amorphous and Liquid Semiconductors** Jaime A. Freitas, Jr.
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This report is a brief overview with commentary of the semiconductors conference held in August 1987 in Prague, Czechoslovakia.

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A brief review of the program of this meeting is given along with comment on the growth in stature of the Spanish work in physics.

Correlation, Orientation, and Spin Effects in Electronic and Atomic Collisions – an ONRL-Sponsored Workshop	Paul Roman	68
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The four principal presentations given at this workshop, held in July 1987 in Belfast, Northern Ireland, are briefly discussed.

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The Nobel Prize Ceremonies For 1987

by Harold Weinstock, Air Force Office of Scientific Research, Washington, DC, Martin Nisenoff, Naval Research Laboratory, Washington, DC, and Alan F. Clark, Office of Naval Research, London. Dr. Clark is the Liaison Scientist for Superconducting Materials and Electromagnetics in Europe and the Middle East for the Office of Naval Research's London Branch Office. He is on leave until March 1989 from the National Bureau of Standards in Boulder, Colorado, where he is Group Leader of the Superconductor and Magnetic Measurements Group.

Introduction

Most scientists choose their profession because they enjoy what they are doing. Yet, like most other human beings, they aspire for recognition which acknowledges they are the best in their chosen field. There can be little doubt that in the physical sciences the ultimate accolade is the award of a Nobel Prize, perhaps the only award which is known and revered by literate people the world over. While the monetary reward which accompanies the Prize is rather significant – about \$340,000 to the each discipline – the awardees achieve a reputation which follows them the remainder of their lives and generally assures them a permanent place in the history of science.

It did not surprise too many scientists in early October 1987 when it was announced by the Nobel Foundation that the Prize for Physics was being awarded to J. Georg Bednorz and K. Alex Müller of the IBM Zurich Laboratory for their discovery of superconductivity up to 36 K in a ceramic oxide, La-Ba-Cu-O. By raising the temperature of known superconductors by about 50 percent after no progress in such activity for 13 years, Bednorz and Müller's singular achievement produced a flurry of excitement and activity in the physics and materials community which is unprecedented. By now it is well known that this activity led to the discovery of even higher transition temperature (T_c) superconductors up to 94 K, with hints of even higher T_c 's all the way to room temperature and above. There are many scientists across three continents who have contributed to this new knowledge, perhaps most notable among them is C.W. (Paul) Chu of the University of Houston. However, since so many of the new discoveries were made contemporaneously, it is surmised that the Nobel Foundation chose to honor Bednorz and Müller for unambiguously "opening the door" which led others to fabricate superconducting ceramic oxides with the T_c 's well above the (77 K) normal boiling point of liquid nitrogen. It is worth noting that interest in the phenomenon of superconductivity and its applications has been high since its discovery in 1911, and the 1987 Nobel Prize in Physics is the fourth to recognize achievement in this field. The first was to Heike Kammerlingh Onnes for the discovery, the second to Bardeen, Cooper, and Schrieffer for their theory, and the third to Josephson, Esaki, and Giaever for tunneling studies.

Being three physicists whose careers have been immersed in the phenomenon of superconductivity, we were genuinely pleased to receive invitations to attend the Nobel Award ceremony and the following dinner on December 10 in Stockholm, and to participate as invited speakers with Bednorz and Müller at a symposium on December 14 at the Chalmers University of Technology, in Gothenburg, Sweden. Our invitations were arranged through the good offices of Professor K.V. Rao (for Clark) of the Royal Institute of Technology, Stockholm, and through the Chalmers University of Technology.

The Ceremony

The invitation to the award ceremony, with a small, raised, gold likeness of Alfred Nobel at the top, informed us that everyone was to be seated by 4:15 p.m. with the program to begin at 4:30 p.m. We already had been informed, prior to receipt of the official invitations, that all male guests were required to wear white tie and tails, a new experience for all of us. The ceremony was held in Stockholm's Concert Hall, a classic structure which features a two-tiered, horseshoe shaped balcony and seats several thousand. As our taxi approached the square in front of the Hall, we were held in place by local police as an entourage of limousines slowly delivered the awardees and their families at the entrance. Crowds lined the street hoping for glimpses of these new celebrities and of the King and Queen of Sweden. At about 3:45 p.m. that afternoon, the sun had set in Stockholm and the temperature was below freezing, but there was excitement, enthusiasm, and a sense of national pride in those lining the square.

Inside the hall was a glittering array of guests: foreign scientists and diplomats, who were permitted to wear native dress, members of the various Swedish academies wearing medals, former Prize winners with a gold medalion around their necks, and about 200 students wearing their nautical white hats and yellow and blue sashes in addition to their formal attire. The stage was elegantly set with flowers, a bust of Alfred Nobel, and a light blue carpet with a large encircled "N" in the center. In tiered seats at the rear of the stage were about 120 members of the

Swedish academies who chose the Prize winners for 1987, and in the balcony behind them was the Stockholm Philharmonic Orchestra. The front sides of the stage were set with ornate chairs for the royal family, the Chairman of the Board of the Nobel Foundation and the five presenters on the right and the eight laureates on the left. These were Bednorz and Müller for Physics, Donald J. Cram, Jean Maria Lehn, and Charles J. Pederson for chemistry, Susumu Tonegawa for Physiology or Medicine, Joseph Brodsky for Literature, and Robert Solow for Economics. The Nobel Peace Prize is given concurrently in Oslo, Norway.

The animated chatter of the audience reduced spontaneously at 4:27 and then, at 4:30 p.m., the hall fell silent, followed shortly thereafter by the entrance of the royal family while everyone rose and the Swedish attendees sang a brief song in praise of the King. The Nobel laureates then were ushered onto the stage to the applause of the audience through a central arch containing the Nobel bust and lined with flowers. Ushering the laureates, who were in white tie and tails, were tall — 6 feet — female students with floor length satin green dresses and the striking blue yellow Swedish sashes across their chests. There was a thrill to this pageantry and to the sense of being in the presence of an assembly of intellectual giants. Words can not do justice to our feelings of awe and excitement.

It came as a bit of a surprise that the entire ceremony takes only about 70 minutes. There was a brief musical interlude by the orchestra between the award(s) for each discipline and a welcoming address to the laureates by the Nobel Foundation Chairman. Then, the Chairman of each prize committee provided about a 5-minute citation on the significance of the achievements of the laureate(s). The opening speech and each citation was presented in Swedish, but a booklet with English translations was provided. Additionally, each presenter concluded the citation by adding a "few words" in the recipient's native tongue, a situation that brought smiles to the audience on the presentation of the Prize in Medicine to Susumu Tonegawa, now a professor at MIT but a native of Japan.

After the reading of each citation, the laureate walked to center stage where he was met by the King, who handed over a plaque and boxed medal in a very formalized ritual. (After shaking hands the King steps back, whereupon the laureate turns slightly to the rear and bows first to members of the academies, then again faces the King and bows to him, and finally faces the audience bowing to his left, center, and right to thunderous applause before he and the King return to their seats for the next musical selection.) The program concluded with the Swedish national anthem and the exit of the royal family and Nobel laureates. Buses then transported audience members invited to the dinner and ball to the Stockholm City Hall, where these events were held.

The Dinner and Ball

About 1,300 people were invited to dine in the courtyard-like Blue Room of the City Hall. The royal party, laureates, and their families entered via a broad marble staircase from the upper balcony level heralded by a pair of elongated and bannered coronets and led by the tall elegant young ladies who appeared in the ceremony earlier. The mood at this function was definitely lighter, and we settled down to a relaxing meal after toasting the winners and Alfred Nobel with champagne. The orchestra entertained us, as did various singers and a ragtag student band in garish dress and full of crazy antics. The one serious period occurred when one of the winners of each Prize was called upon to speak briefly, partly to discuss his work, but mostly to express his feelings and gratitude upon winning the Prize. Although we revelled in the remarks of Alex Müller we could not help being moved by the eloquence of Joseph Brodsky, Robert Solow, and Susumu Tonegawa, the laureates in literature, economics, and medicine.

After dinner, most guests mounted the steps to the Gold Room, which is adorned on all walls with gold mosaic designs and murals, and on this night featured a large dance band. Dancing and relaxing continued well into the night which, along with interviews and comment, were presented live on local television.

The Aftermath

The Nobel laureates have a busy schedule of lectures for a period of several weeks, presenting the "official" Nobel lecture earlier in the week of the award ceremonies to the appropriate academy. On the morning after the ceremony, dinner, and ball, Bednorz and Müller arrived at the Royal Institute of Technology at Stockholm to take part in a panel discussion and answer student questions on the future of superconductivity. With them on the panel were Leon Cooper, a Nobel laureate in 1972 for his contribution to the BCS theory of superconductivity, and Praveen Chaudhari, Vice President for Science at IBM and an active researcher in superconductivity. The student questions are traditionally somewhat irreverent and the discussion that took place was fairly light after the exhausting schedule of the previous several days.

Bednorz and Müller arrived at Chalmers University of Technology in Gothenburg for the symposium just in time for lunch on Dec 14 several days later. To one of us, Alex Müller confessed that he had hoped to have a restful time the previous day (Sunday) but meetings with both students and TV interviewers kept him busy from 7 a.m. to 1 a.m. To another, Bednorz allowed that although the many talks he had to give were similar, that the audiences were always interesting and demanding, especially the one at his own university. When asked if he could take it

easy after the Gothenburg visit, Müller replied that he still had several lectures to give in Norway. Despite this schedule, they listened attentively to the symposium speakers, made extensive comments at their conclusions, and then both gave 1-hour lectures on their past, current, and future research. It was a grueling schedule, but the two 1987 Physics Nobel Laureates appeared to be hold-

ing up well and enjoying their newfound fame. They were exemplary of the outstanding character awarded Nobel Prizes and represented physicists everywhere with competence and dignity.

3/9/88

ACOUSTICS

Natural Mechanism of Surface-Generated Noise in the Ocean A NATO Advanced Research Workshop

by W.A. Kuperman. Dr. Kuperman is a physicist at the Naval Research Laboratory in Washington, DC and an Associate Editor for Underwater Sound of the Journal of the Acoustical Society of America.

The intention of this workshop, held in June 1987 at Lerici, Italy, was to gather together in one room specialists in hydrodynamics, turbulence, cavitation, hydroacoustics, and underwater acoustics in order to discuss the origin and resulting distribution of naturally generated ambient noise in the ocean. Fortunately, the room was not only large enough to accommodate the participants but proved to be an appropriate chamber for the highly spirited discussions which characterized the entire workshop.

Organized by B. Keman, (Atmospheric Environment Service, Downsview, Ontario, Canada), and originally planned as a true "workshop," the popularity of the subject brought out an unexpected plethora of research papers encircling the main topic of the conference. Nevertheless, the organizers managed to maintain the workshop environment, with the result that the meeting was, in my view, extremely successful. No doubt, the proceedings, to be published by Reidel, will be the definitive reference work in this area for many years to come. [A list of the 40-plus formal papers presented, which will appear in the proceedings, is available from the editor, ONRL.]

Because of space limitations, rather than exhaustive review all of the papers, I will instead briefly present the results from the five summarizing workshops.

Wave and Turbulence Noise

The high noise level of about 0.2 Hz (0.1 to 5 Hz) is sea-state related but in a complicated way since it is ob-

served in both shallow and deep water. Candidate mechanisms were not only the wave/wave nonlinear interaction also proposed as the source of microseisms but also atmospheric turbulence or the combined interaction of atmospheric turbulence with the surface wave field. The panel participants concluded that wave/wave interaction was the dominant mechanism, but there were heated discussions concerning the role of turbulence interacting with the surface wave field.

The discussions concerning the region from 5 to 20 Hz were more diffuse, coming to the concrete conclusion that the situation is not clear. The leveling of the spectral slope above 5 Hz is not consistent with wind induced gravity/capillary wave models, and this suggests other sources. Atmospheric turbulence and solitons were possible additional noise source mechanisms discussed.

In the region of 20 to 200 Hz, good propagation conditions result in the contamination of most noise data by long-distance noise sources. This, combined with poor meteorological data associated with noise measurements, results in an uncertain wind dependence on this portion of the spectrum, although at high wind speeds the spectrum level appears to vary as $20 \log(\text{wind speed})$ with n approximately 2.

The mechanisms discussed were: wave/wave interactions, atmospheric turbulence, wave/atmospheric turbulence, oceanic turbulence, gross motions of the sea surface, density discontinuities at the sea surface, bubble convection by turbulence, bubble cloud oscillations, and solitons. Clearly, clever definitive experiments should

The Distribution of Bubbles and Turbulence In and Near a Breaking Wave

The chairman, S. Thorpe (Department of Oceanography, University of Southampton, UK), described this panel's workshop session as "riotous" and said that only the time limit on the session's length prevented violence. Agreed upon was that the basic missing measurement near the ocean surface was the determination on the volume fraction of bubbles as a function of depth and time. How to make this type of measurement inspired much discussion throughout the meeting. Techniques for measuring bubble size distributions, including the optical and acoustical tools, were also discussed. Numerical methods to describe the bubbles and turbulence generated by breaking waves are not yet developed, and laboratory experiments have yet to fully parametrize breaking waves, much less the larger, more complex problem of extending this description to bubble and noise generation.

The experts in this research field agreed on very little, and I had the impression that not only is this a frontier research area but that the direction of the flow of possible fruitful research topics can be in almost any direction. No doubt the proceedings will be a watering trough for many who thirst for new research directions in this field.

Origins of Surface-Generated Ambient Noise at Intermediate and High Frequencies

After briefly addressing the topic of this workshop the chairman, J.E. Williams, steered the discussion to everything of interest, with the result that a very stimulating and lively discussion with main emphasis on hydrodynamics/acoustics ensued. The chairman took issue with wave/wave interaction as the main low frequency source mechanism, stating that phase speeds associated with surface gravity phenomena are so different from those associated with sound propagation that the underwater sound-producing ability of the wind interacting with the ocean surface is a more likely candidate. This invoked an intense dispute.

A suggested important area of research was the radiation of sounds from bubbles near a free surface (causing destructive interference) which has the added complication of being rough. Oceanic spray and rain drops accelerating an inhomogeneous, rough air/water interface were also mentioned as a likely source of strong underwater sound.

Precipitation Noise

The main flow of the discussion in this session was in the direction of suggesting more experiments to accumu-

late a definitive data base concerning the interaction and impact of drops with (complicated) surfaces. It was also pointed out that experiments should examine these phenomena for small drop sizes.

Other experiments were proposed to investigate:

- Drop impacts from larger heights onto random topography
- Effects as a function of drop shape
- Air motion resulting from falling rain drops
- The influence of electric fields on charged drops
- The influence of shear flow in the water surface on the drop impact
- Bubble size distribution as a function of rain
- Salinity effects
- Surface tension effects
- The influence of the angle of drop impact caused by the wind
- The effect of the random timing of the drop impact
- Drop oscillations during surface penetration
- The combined effect of wave breaking and raindrop impacts.

Field experiments were emphasized as being extremely worthwhile but very difficult to design and perform.

Chairman of the session, L. Bjorno (Industrial Acoustics Laboratory, Technical University of Denmark, Lyngby), volunteered to serve as an international coordinator for a common research program in the above areas, emphasizing rain-generated noise in the sea.

Ice Noise

The nature of this area of noise research drove the panel to address observational issues which must: (1) include the widest possible description of the natural environment, (2) be supported by time series of the presumed relevant environmental variations, and (3) be designed to observe the noise and environmental variations over temporal and spatial scales sufficient to resolve the presumed relationship between noise mechanisms and the environment.

The study of heat flux influence on ice fracture resulting in noise radiation was emphasized, and concentration of research in this area in the near term was strongly suggested. Field measurements should investigate the influence of heat flux on thermally induced stress in the ice of ice surface properties in heat transfer to the ice, and of the source of thermal gradients via ice stress considerations and ice crack observations that include the use of acoustic, seismic, and visual techniques.

Laboratory and lake experiment can contribute to this effort if the investigators understand the difference between the properties of natural sea ice and other forms of ice. The elastic plastic plate properties of ice will also be a fertile area for research. Finally, the comment was

made that Arctic ambient noise research is an inverse as well as a direct arena of study and thus that noise measurements can contribute to understanding the physical environment of the Arctic.

Conclusion

This was an extremely lively workshop. The intention to interface researchers concerned with the natural mechanism with those concerned with sound propagation to consider together the ultimate distribution of ambient noise in the ocean was achieved. Though I specialize in sound propagation and ambient noise it was my impression that the more fertile research areas presented were

those concerned with mechanisms. However, it is clear to me that studies of low frequency noise in the ocean must take into consideration sound propagation complexities in order to determine sound levels and directionalities of natural sources. These propagation conditions are simpler in the higher frequency regime.

I already know of at least one research paper that is a result of the existence of this workshop. I have the distinct impression that the success of this workshop will be evident over the next few years as it becomes clear that the workshop and its proceedings will have served as a catalyst for much of the upcoming research in this field.

3/7/88

BEHAVIORAL SCIENCES

Self-Concept and Adjustment Research by Portugal's Adriano Vaz-Serra

by William Crano. Dr. Crano is the Liaison Scientist for Psychology in Europe and the Middle East for the Office of Naval Research's London Branch Office. He is on leave until June 1988 from Texas A&M University, where he is a Professor of Psychology.

The study of self-concept is one of psychology's most important continuing preoccupations. The self-concept, one's assessment of one's own intrinsic worth, is viewed as a central influence on people's behavior. What we think of ourselves has much to do with our beliefs and actions, and with our relations with others. The self-concept permeates every aspect of human life. Accordingly, research on self-concept is not only intense and ubiquitous in psychology, but it is diffused across most of the major subdisciplines of the field. Developmentalists, social psychologists, educational researchers, and clinicians alike have devoted their time and energy to understanding the growth, development, and change of this critical factor which many have viewed as the central feature that distinguishes human beings from all other living creatures. In this report, I will discuss some recent work on the self-concept undertaken in Portugal by Professor Adriano Vaz-Serra and his colleagues. Vaz-Serra is head of the Department of Psychiatry at the University of Coimbra's Hospital Novo, and the Chair of Behavior Therapy in the university's Department of Psychology. He combines a unique set of qualifications – he is both a practicing psychiatrist and a clinical research psychologist – and these qualities are apparent in the

direction, precision, and competence reflected in his work.

Scale Construction: Self-Concept and Coping

This review is divided into two distinct sections. The first is concerned with some of the work that Vaz-Serra has performed in the development of two instruments to measure psychological functions: a *clinical* inventory of self-concept, and a scale devoted to the assessment of the quality of people's coping behaviors. The second section of this report is focused on the empirical relationships found between these two measures, and their subcomponents. In general, the first part of this review might be conceptualized broadly as concerned with issues of reliability; the second with validity.

The Need for a New Scale of Self-Concept

Many measures of the self-concept already exist – in English. Probably the most widely used in the US are the instruments of Rosenberg (1965), Coopersmith (1967), Fitts (1972), Janis and Field (1959), and Marsh, Parker, and Smith (1983). Wiley (1974) has presented a useful

critical discussion of scale construction and validation research in this field. A fair summary of Wiley's remarks would conclude that earlier research on this critical psychological aspect of human beings was hampered by less than adequate measurement technique. More recent endeavors have alleviated these problems somewhat, but there is still a great distance to travel before the importance of the concept is matched by the quality of the research that bears upon it.

In the Portuguese language, the pickings are somewhat more restricted. I am hard-pressed to mention more than a couple of measures of self-concept written in the Portuguese tongue. Tamayo (1981) developed a Portuguese-language scale of self-concept, as have Crano and Crano (1984), but on the whole, the diversity of choice with which the English language researcher is confronted is not encountered in the Portuguese case. This is one reason why Vaz-Serra has developed his own scale of self-concept. Another reason is his conviction, based upon clinical observation, that failures of the self-concept are intimately associated with the problems of anxiety and depression, two of the most commonly encountered maladies with which the psychologist-clinician must contend. It is Vaz-Serra's belief that scale developers should capitalize upon this valuable clinical insight, and construct scales of self-concept that reflect the potential underlying bases of positive or negative self-esteem. His scale, presented later, represents an attempt to do just this. Its aims and paternity are reflected in the title Vaz-Serra applied to it, *"A Clinical Inventory of Self-Concept."*

In discussing the relevance of this work to his practice, Vaz-Serra noted that the ultimate goal of this project was to determine whether variations in self-concept, as measured by his scale, could facilitate treatment of clients with anxiety or depressive disorders. If the scale can identify those who will profit most from one form of treatment, and discriminate these people from those who might do better with another regimen, a major advance will have been made. It is too early to cite research on this goal, but in our discussion, Vaz-Serra seemed well satisfied with progress on these fronts to date. As the review will demonstrate, there are good grounds for such feelings.

Measurement of Self-Concept

Three general approaches have been employed in the measurement of self-concept over the years: behavioral observations, projective techniques, and self-reports. Behavioral observations have been used successfully, but they are time consuming and costly. Projective techniques frequently fail in tests of reliability and validity. By far the most widely used approach to measure self-concept is the self-report, in which a respondent is presented with a self-descriptive item, and asked to indicate the extent to which the item accurately portrays him or her.

Thus, a person might be asked, "How often do you feel that you dislike yourself?" To answer this question, the respondent would be allowed to check one of five possible alternatives, ranging from "very frequently" to "sometimes" to "almost never."

Although scales of this type have been criticized as artificial, in that they do not allow respondents to use their own natural language to describe themselves, the approach has some major advantages: (1) a very complete set of psychometric routines has been developed over the years to allow for the development of measures of high precision and sensitivity; (2) such scales can be scored objectively, thus obviating the effects of scorer bias; (3) the reliability and validity of such scales can be clearly established, and compared with other instruments of the same variety; (4) reasons for the failure of a measurement instrument to operate properly (i.e., reliably) can be identified precisely; and (5) the judicious use of established techniques making use of this information can offset critical difficulties.

Use of natural language measures can render the research subject to all of the problems suggested by the solutions noted in the previous sentence. For these reasons, Vaz-Serra's scale makes use of a standard, fixed set of close-ended questions, and a 5-point response format (such measurement instruments are generally termed Likert scales, after the late Rensis Likert, who first developed measures of this type).

Construction of the Clinical Inventory of Self-Concept

The care lavished on the development of this measure of self-concept is exemplary (cf. Vaz-Serra, 1986) and worthy of discussion. In the initial phases of scale development, Vaz-Serra generated 75 items that he thought might tap some aspect of the self-concept. These were arranged as simple declarative sentences, and administered to more than 500 respondents drawn from the general population. As noted, 5-point response scales were provided, and respondents were to answer all of the 75 items. In the initial item selection, Vaz-Serra was guided by three general criteria:

- Items focused specifically on depression or anxiety were eliminated; since the scale ultimately is to be used to identify the relationship between self-concept and these states, this elimination is a necessity. If this were not done, Vaz-Serra's scale might have been merely an indirect measure of the very states it was developed to predict; the relationship between self-concept, anxiety, and depression could not be studied under such circumstances
- Items were not to tap clinical or seriously abnormal states and feelings, but rather thoughts, feelings, and emotions that a normal individual might experience in

his or her everyday life. So, for example, we would encounter the item "I usually give up when faced with difficulties," but not "I often feel like killing myself."

- Items were written so that approximately equal numbers of positively and negatively worded self-referential statements were used. This was done in order to avoid well known problems of response bias, which can occur if all items in a scale are worded in such a way that consistent acquiescence leads to a consistently high (or low) score on the characteristic under investigation. For example, suppose that all the items of a scale were worded in such a way that agreeing with them would suggest a very positive self-concept. In this instance, a high score could mean either that (1) the respondent did, indeed, have a positive self image, or (2) that he or she had a strong tendency to acquiesce to positively worded statements. In the second instance, such a tendency actually would be negatively related to positive self-concept, yet the competing response tendency would mask the true relationship. Accordingly, as a matter of course, good measures of personality or attitudes should contain approximately equal numbers of positively and negatively worded items.

After the first administration, which was undertaken *not* to measure the self-concept of the 500-plus respondents, but to assist in the choice of the best trait-descriptive items, Vaz-Serra used the following criteria to decide upon the items to be retained in the final version of the scale:

- First, he first eliminated all items whose meaning appeared ambiguous on the basis of the obtained data.
- Second, he eliminated all questions that did not correlate positively with the total score. This is standard practice. It is based on the assumption that the total score, albeit imperfect, is the best estimate of the underlying dimension of interest. As such, items that correlate most strongly with this estimate are assumed to be better (i.e., more sensitive indicants of the dimension) than those that do not.
- Third, he eliminated those items that appeared not to discriminate between groups of respondents that had been formed on the basis of the extremity of their total scale score. To do this, Vaz-Serra calculated all the total scores of all subjects by summing their responses to all retained items. The extreme quartiles of the resulting distribution were identified. Then, items that appeared to be answered differently by the extreme groups were retained.
- Finally, he eliminated all items that were answered differently by men and women. Since Vaz-Serra's aim is to create a general scale equally applicable to both sexes, this tactic makes good sense.

A total of 31 items remained after all of these operations. After a factor analysis (see Table 1), yet another technique used to facilitate the choice of the most useful items, Vaz-Serra identified the 20 questions that were

most likely to produce a good result. I have presented the English translation of the items constituting this scale in Table 1.

Table 1. Translated Items of Vaz Serra's Clinical Inventory of Self-Concept

1. I know I am a likeable person.
2. I usually am honest when expressing my opinions.
3. I usually give up when faced with difficulties.
4. When meeting other people, I usually am talkative.
5. As a rule, I am quick in completing the tasks I have to do.
6. I consider myself tolerant towards other people.
7. I am capable of assuming responsibility for something until the end, even though it may have unpleasant consequences.
8. Generally speaking, I usually face my problems and solve them.
9. I usually am well accepted by others.
10. When I have an idea that seems to be good, I like to make it work.
11. As a rule, I am persistent in solving my problems.
12. I don't know why, but most people pick on me.
13. When I am questioned about important matters, I usually tell the truth.
14. I consider myself competent in what I do.
15. I am the kind of person who loves to do what I like.
16. The way I am makes me feel reasonably well adapted to life.
17. I consider myself a pleasant person to get on with.
18. When I have a problem that worries me, I cannot solve it without help from other people.
19. I like to succeed in the things I undertake.
20. I always find energy to overcome my problems.

Response Options: "Strongly disagree, disagree, neutral, agree, strongly agree."

This set of 20 items was then administered to an additional 920 respondents. The coefficient of internal consistency (i.e., the extent to which the items "hang together") reported by Vaz-Serra (1986) on this administration, across all 20 items, was strong (coefficient $\alpha = 0.77$). This is an important consideration because the typical practice is to sum scores across items in order to arrive at the best estimate of the critical dimension—in this instance, self-concept. If the items are unrelated, their summation makes no logical sense. In the present instance, however, the items all appear to tap the same dimension of self-evaluation.

Temporal stability of the instrument also is strong. Test retest reliability in a sample of 108 respondents, with test administrations separated by at least 1 month, was 0.84.

In an attempt to develop a more fine-grained instrument, Vaz-Serra factor-analyzed the matrix of correlations between the 20 items. Factor-analysis is a multivariate analytic technique whose aim in this instance is to reduce the data set by finding items that are mutually and highly interrelated with each other, and minimally associated with others. Interrelated items are said to form a "factor," and such factors provide the basis for constructing subscales in personality or attitude surveys.

Subscales allow the researcher to assess individuals with greater degrees of precision than that possible when the entire gross item set is employed.

Vaz-Serra's factor analysis (for those technically inclined, he used a principal components analysis with Varimax rotation) of the matrix of responses obtained on the major sample of 920 respondents revealed a six-factor solution, four of which were psychologically meaningful. That is, six distinct clusters of items were isolated by the analysis, and of these, the items of the first four could be interpreted sensibly. Vaz-Serra reports his first factor as being composed of items 1, 4, 9, 16, 17 from Table 1. He interprets this factor as representing a dimension of social acceptance or rejection. On the basis of his published data, I calculated the coefficient of internal consistency of these items. It was of reasonable magnitude (coefficient $\alpha = 0.68$).

The second factor reported by Vaz-Serra (items 3, 5, 11, 18, 20) appears to focus on self-efficacy. Internal consistency of the five items is of marginally acceptable magnitude (coefficient $\alpha = 0.63$). Crano and Brewer (1986) have suggested a minimum acceptable internal consistency coefficient of 0.70.

The internal consistencies of the items constituting the two remaining interpreted factors are not, in my opinion, of sufficient magnitude to inspire confidence in their utility. (Subsequent research by Vaz-Serra will bear this out.) Factor 3 (items 2, 6, 7, and 13), for example, is thought to tap psychological maturity. Although the items constituting this factor appear related at the linguistic level, their degree of interconnectedness inferred from the actual data is not great (coefficient $\alpha = 0.48$). In part, this is due to the small number of items constituting this subscale. Statistically, it is possible to estimate that if 10 items were used in the construction of this subscale, the coefficient of internal consistency would approximate 0.70 if the extent to which the present items are interrelated was maintained.

The fourth factor (items 10, 15, 19) is thought by Vaz-Serra to measure impulsivity or activity. As with the third set of items, the coefficient of internal consistency of this three-item subscale is lower than one would wish (coefficient $\alpha = 0.54$). Doubling the number of items in this subscale and maintaining the same degree of interrelatedness would result in a coefficient of internal consistency of 0.70.

An Early Evaluation. The items constituting Vaz-Serra's "Clinical Inventory of Self-Concept" should not be conceptualized as written in stone. The work discussed here is best seen as a description of the initial attempts to construct a useful and usable tool. The translated version of these items in Table 1 is included to provide the starting point for the reader who might wish to extend Vaz-Serra's work on an English language version of this measure. Obviously, the subscales formed to this point

are far from perfect. At a minimum, more items should be added to each in order to enhance internal consistency. However, the present items form the basis of a good working scale whose potential utility seems high. In his own clinical practice, for example, Vaz-Serra has noted that psychiatric patients scoring high on the first factor, which is focused on social acceptance or rejection, typically display psychological disturbances associated with anxiety, most especially social anxiety. Those whose scores lie near the top of the distribution of scores on the second (self-efficacy) factor are more likely to display clinical depression. These relationships were expected on the basis of item content. Discovering such results in an actual clinical population is noteworthy. If a more refined instrument were developed, we might be able to produce some remarkably useful clinical insights.

Construction of the Problems-Resolution Inventory

Vaz-Serra employed psychometric approaches similar to those he used in the development of the self-concept instrument in constructing a new measure of coping skills. Measures of coping skill are practically nonexistent in the Portuguese language. So, at a minimum, the development of a successful coping skills inventory represents a major contribution. But Vaz-Serra has more in mind. In his experience, coping skill and self-concept are intimately connected. As a practicing psychiatrist, he intends to learn if this insight is borne out statistically. Then, if all goes well, it is reasonable to assume that he will try to determine the causal connections that link these two factors. Is a low self-concept a consequence of poor coping skills, or does poor coping ability lower the self-concept? If through our therapy we enhance self-concept, does this influence subsequent coping skills? Can an enhanced self-concept be maintained in the face of poor coping abilities, or is it more reasonable to focus our therapeutic attention on the training of coping responses, on the assumption that a more positive self-concept is the almost inevitable result of such training? Questions of this type demand the ability to measure both self-concept and coping in an objective, reliable manner, and it is to these goals that Vaz-Serra's work is directed.

In Folkman's (1984) view, to which Vaz-Serra subscribes, coping is defined as "the cognitive and behavioral efforts used by the individual to master, reduce, or tolerate the internal or external demands that are created by stressful interaction." People cope in many ways, of course, but in general, most coping strategies reduce to: (1) people's attempts to alter the relationship or environment that is the cause of the trouble, or (2) the attempted reduction of the emotion that is experienced in response to the problem (cf. Fisher, 1986; Lazarus, 1966). In the

first strategy, the individual attempts to correct the problem by direct confrontation and resolution. The second option, reduction of felt emotion, can be accomplished through intrapsychic processes (ego defense mechanisms) and by somatic devices, such as drugs, alcohol, biofeedback training, etc.

Use of either type of coping tactic can be costly, and success or failure has major implications for mental health. This is reason enough for a psychiatrist to be interested in this phenomenon. Another reason acknowledges the commonly observed fact that some people can tolerate high degrees of stress while others cannot. What distinguishes such people? Could the self-concept be implicated? To investigate these possibilities, Vaz-Serra has embarked on the difficult task of developing an inventory whose function is to distinguish people in terms of the varieties and relative effectiveness of their coping abilities. Even more than this, he is attempting to determine whether people are better at one form of coping than another, and if so, what the implications of these differences are for mental health. This is not a modest goal, but a good start has been made. So without further adieu, let us consider Vaz-Serra's work on the coping inventory.

In his coping skills test (the Problems Resolution Inventory [PRI]), Vaz-Serra presents respondents with three scenarios having to do with threat, loss, or challenge. Following each scenario is a (different) set of questions asking the respondent to estimate his or her likely response. As in the self-concept measure, a five-point response format is employed, thereby constraining subjects' responses to one of five possibilities on each item. One of these scenarios follows:

Imagine you had a serious argument with an old friend. You owe him a great deal of money, which should already have been repaid, as well as other favors. You have many acquaintances in common. In the argument that took place, you were in the right. However, the other person became very angry and eventually told you: "I give you a week to think about what you did to me and apologize. If you don't, I shall tell everybody that you are a swindler and I shall demand that you repay me in full."

Deep inside, you are practically convinced that the other person is capable of doing what he said. You also know that you do not have enough money to repay your debt. You are certain that many of the friends you have in common may believe in whatever the other person tells them. This situation may go on for some time, involving persons with whom you are in daily contact.

The dispute would come to an end if you had a serious talk with the other person, during which you could clarify, once and for all, your misunderstandings. Such a talk could well be unpleasant, at least in the beginning. But it is possible

that you would be friends again, as you were in the past, and the debt problem would be postponed. However, you would have to recall what took place. On one hand, you took offense at the other person's attitude; on the other hand, you fear the possible consequences. You don't really know how to solve that problem.

In a situation of this kind, you are likely to think:

1. I shall leave the dispute to itself; time will help clear up the problem.
2. The best I can do is avoid meeting the other person, and pay no attention what he/she may do or say.
3. I shall not allow this event to interfere with my daily activities, etc.

Five-point scales are provided to allow respondents to note the extent to which they agree or disagree with the various options presented.

After the initial phases of scenario choice, culling bad or ambiguous items, etc., the 40-item inventory was administered to 588 respondents from the general population. The resulting response set was factor analyzed, and a nine-factor solution obtained. These results are interesting because they cover the gamut of coping mechanisms that people employ when reacting to threat, loss, or challenge. Vaz-Serra's descriptive summary of the items that constitute the factors follows:

- Factor 1. Seeking help
- Factor 2. Confrontation and active resolution of the problem
- Factor 3. Passive Abandonment of the situation
- Factor 4. Internal/external control of problems
- Factor 5. Strategies for the control of emotions
- Factor 6. Nonintervention – waiting-out the problem
- Factor 7. Internalized/externalized aggression
- Factor 8. Self-blame and fear of consequences
- Factor 9. Confrontation with the problem and planning a response.

In an investigation of temporal stability on the total scale, Vaz-Serra found test-retest reliability to be very strong ($r_{11} = 0.81$). Coefficients of internal consistency of the items constituting the nine item-clusters extracted in the factor analysis were not reported. However, given the rather limited number of items employed to define each factor, it is unlikely that many of the internal consistency coefficients of the various subscales are of acceptable magnitude. Even so, the results to date are encouraging. Vaz-Serra has made an impressive start on the development of a measure of coping efficacy. The utility of this instrument is demonstrated in the following section, in which research on the relation between self-concept and coping is discussed.

Self-Concept and Coping

In one of his first studies making use of both instruments, Vaz-Serra gathered data on a total of 588 respondents (276 men, 312 women). Before beginning these measures, all respondents had to indicate whether they had ever suffered any serious mental disturbance – in layman's language, a "nervous breakdown." This variable, along with sex, was used to subdivide the sample further into "normals" (N = 418 [226 men, 192 women]) and "abnormals," (N = 170 [50 men, 120 women]).

Relations between Self-Concept and Coping. Table 2 summarizes the correlations between the various subscales of the self-concept and the coping inventories. The correlational data indicate a very strong, positive association between the total scores of the coping and self-concept inventories. Clearly, the two measures are related, at least at the most gross level. The second subscale of the coping inventory, which taps "confrontation and active resolution of problems," also correlates significantly with self concept scores. Vaz-Serra views active confrontation as the most important of all the coping mechanisms assessed in his inventory, so this strong relationship is encouraging. Indeed, this subset of the coping inventory correlates significantly with all four of the subscales of the self-concept measure.

Table 2. Relationships between coping and Self-concept measures: total and subscale scores.

Coping Scale	Total Score	Self-Concept			
		Sub Scale 1	Sub Scale 2	Sub Scale 3	Sub Scale 4
Total Score	.558	.301	.619	.342	.319
Subscale 1	.133	-.068	.284	.098	-.013
Subscale 2	.609	.371	.589	.427	.463
Subscale 3	.153	.072	.181	.121	.082
Subscale 4	.344	.233	.404	.162	.111
Subscale 5	.045	-.031	.149	-.028	.329
Subscale 6	.397	.296	.312	.280	.329
Subscale 7	.178	.087	.184	.124	-.001
Subscale 8	.279	.174	.277	.160	.143
Subscale 9	.333	.209	.325	.159	.291

Note: For $r > .15$, $p < .001$.

Of the self-concept measures, the second subscale (self-efficacy) looks most promising. The sum of the items thought to tap self-efficacy correlates significantly with all nine of the coping subscales. These results are very impressive because it is well known that if a scale (or subscale) is of low reliability, its correlations with other variables will be attenuated. The present results suggest that enhancing the reliability of one or both of the instruments would have a powerful influence on the observed associations between the total scores and the various subscales of these two interesting scales.

Normals vs. Abnormals. As a rough and informal check on the validity of the coping inventory, Vaz-Serra asked respondents to tell him whether they had ever in the past experienced a severe psychological problem. He then compared the self-concept and the coping scores of those categorized on the basis of their answers. Table 3 contains a summary of these comparisons. As shown, the classified subjects differed on the self-concept inventory only on the self-efficacy subscale. Self-efficacy self ratings of respondents who claimed to have had a severe problem were significantly less than those who did not.

Table 3. Mean differences between normal and abnormal respondents on coping inventory total and subscale scores

Coping Scales	Normal	Abnormal	t	p <
Total Score	158.84	136.06	15.10	.001
Subscale 1	17.57	15.36	4.97	.001
Subscale 2	25.49	21.51	8.08	.001
Subscale 3	13.34	12.28	4.82	.001
Subscale 4	32.88	26.66	13.18	.001
Subscale 5	17.66	13.03	17.34	.001
Subscale 6	13.50	12.43	3.40	.001
Subscale 7	9.58	8.79	5.96	.001
Subscale 8	16.94	15.04	6.20	.001
Subscale 9	11.88	10.96	4.27	.001

On the coping inventory, significant differences were found between the two groups on four of the nine subscales, and on the total score. In every comparison, the "normal" respondents had better coping scores than the "abnormal" group. This is noteworthy because Vaz-Serra did not take into account the recency of the problems that respondents in the abnormal group claimed to have suffered. For some, the difficulty might have occurred many years ago, and they long since presumably had recovered from it. In addition, it is conceivable that some in the "normal" group had misidentified themselves, for reasons of self-presentation. Accordingly, if anything, the methodology of this study would tend to underestimate differences between the two groups on coping effectiveness.

Future Directions

The data presented to this point are intriguing. Vaz-Serra has been able to discover some powerful relationships between aspects of coping and self-concept despite using scales and subscales of marginal reliability. What should be done next? If I were working on these issues, I would undertake a systematic series of research operations to capitalize on the important progress that has been made to this point. The first order of business would be to enhance the reliabilities of the subscales that constitute the two measures. The standard way of doing this is to add more, and relevant, items to the subcomponents, and thereby produce measurement devices that more precisely

ly pinpoint the factor that is under consideration. In some cases, the addition of merely two or three items would make a major impact on the internal consistency of the subcomponent, which in turn would almost inevitably enhance its predictive power.

Having boosted internal consistency reliabilities, it would then be useful to study temporal stability. We know from Vaz-Serra's earlier studies that the test-retest reliabilities of the total scores of the two measures were of acceptable magnitudes. But it is important that the test-retest correlation also prove strong at the level of the subscales. Enhancing internal consistency of the subcomponents (step 1, above) will have positive implications for their temporal stability as well.

Having established two reliable measurement instruments, it would be appropriate then to inspect the validity of the measures. That is, having established that we have scales that measure something reliably, we would then want to be sure what that "something" was. The method of construct validation, in which the new measures are compared with results of established instruments, is an obvious choice. Criterion validation would also help to establish the utility of the scale. To study criterion validity, we hypothesize that on the basis of prior theory or experimentation, subjects classified differently on a measuring instrument should act differently. If this expectation is confirmed, our confidence in the measurement devices is enhanced. In the present instance, we could measure respondents on either the self-concept or coping inventory (or both), and place them in situations in which the behavior of highly self-confident (or people with good coping ability) would be expected to differ from that of people who lack confidence. If respondents identified by the scale responded in the ways predicted, confidence in the validity of the scale would be enhanced.

Assuming all goes well to this point, we are now in a position to study the relationship of psychiatric patients' scale scores with their presenting symptomatology. This was, in fact, one of the principal motivations for the development of the instruments. For Vaz-Serra, it is critical to know if specific psychological disorders are associated with different patterns observed among the various subscales of his self-concept and coping inventories. If such proves to be the case, then the next round of research will search for relationships between scale

scores, maladies, and responsiveness to variations in treatment regimens. Assuming that some useful information is derived from such study, we will be in a position to develop a formal theoretical model of relationships among self-concept, coping, pathology, and cure. This is not a modest ambition, but a wonderful start has been made, and there is no doubt that a successful conclusion to this research series will more than offset the tremendous investments that will have to be made to arrive at this happy point.

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1/28/88

Forthcoming European Conferences in Psychology

The First European Congress of Psychology will be held from 2 through 7 July, 1989, in Amsterdam, The Netherlands. It will be organized by the Dutch Institute of Psychologists and the Dutch Foundation for the Advancement of Psychological and Psychoeconomic Research,

together with the European Federation of Psychological Associations, and under the auspices of the International Association of Applied Psychology. The conference will focus on every aspect of European Psychology as a science and as a profession. Social psychology will be em-

phasized, and treated as the central topic. For information, write to Secretary of the first European Congress of Psychology, B.P. 71275, 1008 BG Amsterdam, The Netherlands.

A Conference on Social Justice and Societal Problems will be held from 1 through 3 August, 1988, in Leiden, The Netherlands. The conference will be organized around 11 thematic sessions, including:

- Social policy and welfare institutions
- Justice and the family
- Procedural justice and legal institutions
- Intergroup relations, cooperation and competition
- Life crisis, societal victimization and redundancy
- Income distribution and social stratification
- Justice in the workplace
- International relations
- Political economy and decision making
- Methodological issues in justice research
- Emancipation and affirmative action.

Requests for information should be to Dr. R. Vermunt, Department of Psychology, University of Leiden, Hooigracht 15, 2312 KM Leiden, the Netherlands.

The seventh annual conference of CHEIRON-Europe (European Society for the History of the Behavioral and Social Sciences) will be held in Budapest, Hungary, from 4 through 8 September 1988. Papers dealing with any aspect of the history of psychology, and with the philosophical and methodological problems of historiography, will be presented. Three symposia are planned:

- Vygotsky and his thought in the history of psychology
- Psychoanalysis in the Central European context
- Racism, eugenics, and the social sciences.

Enquires should be addressed to Dr. Ferenc Eros, Hungarian Academy of Sciences, Szondy u. 83-85, H-1394 Budapest, Hungary.

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1/28/88

BIOLOGICAL SCIENCES

Medicinal Chemistry Symposium Cambridge, UK

by Claire E. Zomzely-Neurath. Dr. Zomzely-Neurath is the Liaison Scientist for Biochemistry, Neurosciences, and Molecular Biology in Europe and the Middle East for the Office of Naval Research's London Branch Office. She is on leave until July 1989 from her position as Director of Research, the Queen's Medical Center, Honolulu, Hawaii, and Professor of Biochemistry, University of Hawaii School of Medicine.

Introduction

The 4th SCI-RSC Medicinal Chemistry Symposium was held at Churchill College, Cambridge, from 6 through 9 September 1987. The conference was organized by the Fine Chemicals Group of the Society of Chemical Industry, and the Royal Society's Industrial Division and the Fine Chemicals and Medicinals Group. Of the 240 participants 74 percent represented industrial organizations with the balance from academic institutions. Although the majority of attendees were from the UK, an appreciable number came from eight West European countries as well as from the US, Canada, and Japan. The format of the scientific program consisted of five plenary lectures, oral presentations, and poster sessions. The following topics were covered in this timely and focused conference:

- Neuropeptides

- Control of enzymatic processes in medicinal chemistry
- Antiviral agents
- Antibacterial, antifungal, and antiparasitic agents
- Application of computing to medicinal chemistry.

This conference was intensive in its coverage of these topics. Therefore, only summaries of selected presentations can be given in the following report. However, the proceedings of the meeting will be published in the near future as a Royal Society of Chemistry Special Publication.

Neuropeptides

The subject of multiple receptors for substance P (SP) and related tachykinins was discussed by L.L. Iversen (Merck Sharp and Dohme Research Laboratories,

Neuroscience Research Center, Harlow, UK). The tachykinins are a family of naturally occurring peptides which share a common C-terminal sequence: -Phe-X-Gly-Leu-MetNH₂. The mammalian peptides are SP, neurokinins A and B. Iverson stated that it is now clear that the biological actions of the tachykinins are mediated by more than one receptor subtype in mammalian tissues. Recent work by Iverson and his group suggests that as many as four receptor subtypes can be distinguished. These are:

1. NK-1. NK-1 receptors are present in smooth muscle (guinea pig ileum), glandular tissues (rat parotid), and brain. This is the only receptor for which SP has high affinity although other tachykinins (eledoisin, neurokinins) are also recognized for high potency. SP methyl ester is a highly selective agonist, and the sites can be radiolabeled with I¹²⁵-BH-SP.

2. NK-2. These receptors are present mainly in the urinogenital system (hamster bladder, rat vas deferens). The NK-2 receptors have thus far not been found in the central nervous system. Neurokinin A is the preferred natural agonist (100 times more potent than SP). (G1p⁶, D-Pro⁹) SP₆₋₁₁ is a potent agonist, but the corresponding L-Pro⁹ analog is inactive (the reverse selectivity is seen at NK-1 sites).

3. NK-3. These receptor sites are present in the central nervous system (CNS), especially cerebral cortex, and in peripheral neural (myenteric plexus) and smooth muscle (rat portal vein) preparations. Neurokinin B is the preferred agonist (almost 500 times more potent than SP). The synthetic analog "senktide" Suc-(Asp⁶, NMe-Phe⁸, Sar⁹) SP₆₋₁₁ is a highly selective agonist. The NK-3 sites in brain can be radiolabeled by I¹²⁵-BH-eledoisin.

4. NK-4. NK-4 is a recently described subtype presently known to exist only in air passages (guinea pig trachea). There is no particular preference for a naturally occurring mammalian tachykinin, though neurokinin is most potent. The synthetic compounds DiMe-C7 = (G1p⁵, NMePhe⁸, Sar⁹) SP₅₋₁₁ and L-363,851 = G1p-Phe-Phe-(R) Gly [ANC-2]-Leu-MetNH₂ are highly selective and potent agonists.

Iverson emphasized that the area of tachykinins has become increasingly complicated as research progresses, and some indication of this complexity is seen above. The tachykinins have a great potential for eventual medical application since they have many and diverse biological effects. For example, SP is involved in the contraction of smooth muscle and also exhibits vascular effects such as hypotension and vasodilation. In addition, SP appears to be involved in the stimulation of secretion by salivary glands and pancreas as well as excitation of neurons.

Modification of Peptidergic Neurotransmission. Novel approaches to the pharmacological modification of peptidergic neurotransmission were discussed by B.P. Roques (Department of Organic Chemistry, Inserm Unit

498, CNRS and Division of Pharmaceutical and Biological Sciences, Paris, France). Roques said that in the CNS, neuropeptides such as enkephalins, CCK, SP, etc. behave both as classical neurotransmitters interacting with postsynaptic receptors to ensure the transmission of the nerve impulse and as neuromodulators acting presynaptically to modulate the release of various effectors (monoamines or peptides). As illustrated in the case of CCK and dopamine (DA) in the mesolimbic pathway, neuropeptides are also able to modify the threshold of the physiological responses induced by the colocalized neurotransmitter. Furthermore, the interruption of the actions induced by interaction of neuropeptides with various receptor types is ensured by more or less specific peptidases which, according to Roques, cleave the native peptide into inactive fragments. Analysis of the physiological relevance of a given neuropeptide requires the use of molecules (agonists or antagonists) interacting selectively with the different receptor types. Roques said, moreover, that the occurrence of a physiological control of the responses induced by stimulation of the various types of receptors through a tonic (or phasic) release of neuropeptides can be investigated by inhibition of their degrading enzymes.

Such a strategy has been followed by Roques and his group to study the respective role of the enkephalins and the sulfated octapeptide CCK-8 in the brain. Agonists highly selective for μ (TRIMU 5) and δ (DTLET, DISTUBLET) opioid receptors and for central CCK binding sites were rationally designed by taking into account the conformational properties of the native peptides. Likewise, highly potent and specific inhibitors of the various enkephalin-degrading metallopeptidases (neutral endopeptidase or NEP), aminopeptidase M, and dipeptidylaminopeptidase) were synthesized by Roques and his group using as a model the structure of the active site of thermolysin, a bacterial endopeptidase which has been crystallized either alone or in the presence of various inhibitors. Roques said that the relevance of this approach is supported by the similarity in the three-dimensional arrangement of amino acids in the active site of thermolysin and NEP, the sequence of which was recently determined from its cloned complementary DNA (cDNA). Using this approach, Roques and his group synthesized NEP inhibitors such as thiorphan and retro-thiorphan and mixed bidentate inhibitors such as kelatorphan, a compound able to completely inhibit *in vivo* enkephalin metabolism. Computer graphic analysis was of great value, according to Roques, for the exploration of (1) the conformational arrangement for optimal interaction of R and S retro-thiorphan with NEP and (2) the stereochemical requirements of peptide analogs to fit by a "zipper" mechanism μ or δ opioid binding sites or CCK receptors. Finally, tritiated analogs of these probes were extensively used to determine the distribution of NEP and

of various receptor types in the CNS by radioautography. Also, this technique was used to study the plasticity of neuropeptidergic targets either after lesions of brain structures or after pharmacological treatments.

Roques said these studies were essential for determining—after local administration of agonists, antagonists, or kelatorphan—the types of receptors involved in a given response as well as the occurrence of a tonic or phasic control of the response by the endogenous peptides. Roques and his group found that μ receptors are crucially implicated in supraspinal pain control while μ and δ agonists behave independently as analgesics in the spinal cord. At both levels, nociceptive stimuli are tonically controlled by enkephalins. In the mesocorticolimbic pathways the endogenous opioid peptides were also crucially involved in the control of locomotor activity and exploratory behavior, with a major role played by the receptors. In contrast, no tonic control by enkephalins was observed at locus coeruleus and N. tractus solitarius levels. Roques stated that the use of CCK analogs highly selective for central receptors emphasized the major role of CCK-8, that acts in opposition to enkephalins in various DA-innervated brain structures.

In addition to their specific actions (analgesia for enkephalins, inhibition of food consumption for CCK-8) the putative therapeutic interest of these neuropeptides could be their ability to function as "physiological regulators" of monoaminergic pathways and consequently in their involvement in cognitive function and integration of sensorimotor messages, according to Roques.

Restriction in Opioid Peptides. Pharmacological consequences of conformational restriction in opioid peptides was discussed by P.W. Schiller (Clinical Research Institute of Montreal, Canada). In an effort to reduce the conformational flexibility of linear opioid peptides, Schiller and his group synthesized cyclic analogs. Various types of cyclic enkephalin analogs were obtained through side chain to end group cyclization (for example, H-Tyr-D- Lys-Gly-Phe-Leu) or through cyclization between two side chains of appropriately substituted amino acid residues (for example, H-Tyr-D- Cys-Gly-Phe-Cys-OH (or NH₂) or H-Tyr-D- Lys-Gly-Phe-Glu-NH₂). The *in vitro* opioid activity profiles of the analogs were determined with μ - and δ -receptor representative binding assays and bioassays. Several cyclic analogs showed high preference for μ -receptors and comparison with corresponding open-chain analogs revealed that the μ -receptor selectivity was a direct consequence of the conformational restriction resulting from ring formation.

Schiller and his group found that various types of amide bond replacements within the ring structure of some of the cyclic peptides produced either an increase or decrease in receptor selectivity. In comparison with their linear correlates, several cyclic analogs had lower

μ -receptor affinities but considerably higher potencies in μ -receptor representative bioassays. Schiller said that this discrepancy may be due to an enhanced "efficacy" ("intrinsic activity") of the cyclic peptides.

The results of parallel structure-activity studies indicated that cyclic and linear opioid peptide analogs have the same mode of binding to the receptor but differ from one another in the binding process—i.e., "lock-and-key" versus "zipper"-type interaction. Furthermore, Schiller and his group demonstrated that the cyclic enkephalin analogs were highly resistant to enzymatic degradation and that they were able to produce a long-lasting analgesic effect after intravenous administration.

Schiller also discussed conformational features of several cyclic analogs on the basis of results obtained from nuclear magnetic resonance (NMR) spectroscopic studies and theoretical energy calculations.

"Peptoids." The subject of "peptoids" (orally bioavailable peptide mimetics) from CCK-8 was discussed by D.C. Horwell (Parke Davis Research Unit, Addenbrooke Hospital Site, Cambridge, UK). He presented a rationale for designing "peptoids" from biologically active peptides. This involved examination of both continuous and noncontinuous fragments of the peptide in a binding assay to establish the minimum acceptable fragment, followed by demonstration of the agonist/antagonist profile and then optimization of the pharmacokinetic properties by chemical modification.

CCK-8 (CCK 26-33) has been shown to be the minimum fragment of CCK that retains both peripheral and central cholecystokin-like activity. Using a mouse cerebral cortex assay Horwell and coworkers found that CCK-4 (CCK 30-33) is the minimum fragment that retains nanomolar binding affinity for the central CCK receptor, using both (¹²⁵I)-CCK-8 and (³H)-Boc-B-alanyl-CCK 30-33 (pentagastrin) as label. Structure-activity relationships from binding data with both continuous and noncontinuous fragments revealed that the tryptophan and phenylalanine residues together formed the minimum essential fragment required for receptor recognition—i.e., Boc-Trp-(CH₂)_n Phe-NH₂, where n = 0,1,2.

Control of Enzymatic Processes in Medicinal Chemistry

Renin Inhibitors. Studies on renin inhibitors were reported by A. Wagner (Hoechst AG, Frankfurt, West Germany). The renin-angiotensin system (RAS) is a complex, mixed enzymatic-hormonal system controlling electrolyte balance, blood volume, and arterial blood pressure. It consists of two main enzymes, the highly specific renin, and angiotensin-converting enzyme, which finally produce the potent vasoconstrictor, angiotensin II. Renin, an aspartic protease, catalyzes the first and rate-limiting step within this cascade to yield the inactive an-

giotensin I. Wagner said that pharmacological interruption of the RAS by converting enzyme inhibitors (for example, captopril, enalapril) has proven to be of great therapeutic value in the treatment of high blood pressure. This has, according to Wagner, encouraged intensive search for inhibitors of the more specific renin. To date, two main structural classes of inhibitors have been established: (1) substrate, or reduced substrate analogs, derived from the segment of the natural substrate angiotensinogen, and (2) transition-state analogs, containing a hydroxyethylene moiety in place of the scissile bond. So far, the metabolic lability, common to many peptides, limit their use as drugs, according to Wagner. This fact has concentrated most of the synthetic effort on altering the peptide backbone, with the goal of producing small or nonpeptidal renin inhibitors. Structure-activity studies of transition-state analogs, derived from statine, have led Wagner and his group from potent and orally active tetrapeptides to the study of dipeptides, which is currently the research emphasis of this group.

Design of Enzyme Inhibitors. The topic of the rational design of enzyme inhibitors containing small rings was discussed by C.J. Suckling (Department of Pure and Applied Chemistry, University of Strathclyde, Glasgow, UK). The observation several years ago that horse liver alcohol dehydrogenase recovered its activity on standing after inhibition with α,β -unsaturated aldehydes led Suckling and his group to propose that the ring-homo system, namely cyclopropyl aldehydes, would act as inhibitors if the electrophilicity of the cyclopropane ring could be enhanced by increasing the polarization of the carbonyl group. Studies with alcohol dehydrogenase confirmed this expectation. Suckling and his coworkers then undertook a research program in which the extent of applicability of this enzyme inhibiting device was examined. These investigators hypothesized that the small cyclopropane ring could be transposed into many enzyme substrates to generate inhibitors activated by the enzyme. Suckling and his group evaluated their hypothesis with reference to lactate dehydrogenase, cytochrome P-450 type enzymes, dihydrofolate reductase, carboxypeptidase A, and other peptidases as well as dihydroorotate dehydrogenase. They found inhibitors of all these enzymes except for cytochrome P-450. Suckling discussed their properties and possible mechanisms of interaction with their target enzymes. Suckling and his group are carrying out studies for extending the strategy of using small rings to generate specific enzyme inhibitors.

Amino Sugar Derivatives. The subject of amino sugar derivatives and related compounds such as glycosidase inhibitors was discussed by G.W.J. Fleet (Dyson Perrins Laboratory, Oxford University, UK). He said that replacement of the pyranose oxygen of a sugar by nitrogen leads to a class of specific and powerful

glycosidase inhibitors. Thus the naturally occurring manno-jirimycin, nojirimycin, and galactostatin are inhibitors of mannosidases, glucosidases, and galactosidases, respectively. Removal of the anomeric hydroxyl group gives a more chemically stable class of compound with powerful and specific glycosidase inhibitory properties. Fleet stated that bicyclic compounds containing polyoxygenated piperidines and pyrrolidines such as castanospermine and swainsonine are also glycosidase inhibitors. Several naturally occurring azafuranose derivatives have also been shown to be enzyme inhibitors. It has also been found, according to Fleet, that synthetic analogs of other aza sugars provide opportunities for the design of specific inhibitors for other glycosidases.

Fleet discussed the preparation by his group of both synthetic and naturally occurring polyhydroxylated monocyclic and bicyclic compounds containing pyrrolidines and piperidines with some indication of the ability of these compounds to inhibit glycosidases. However, Fleet primarily discussed various strategies for the synthesis of these compounds from carbohydrates. He also presented a method which can easily be used for the synthesis of about 10 to 15 grams of deoxymanno-jirimycin as well as presenting some preliminary studies on the synthesis and properties of the corresponding 6- and 5-ring lactams.

Antiviral Agents

The topic of novel synthetic methods for antiviral agents was addressed by S.M. Roberts (Department of Chemistry, University of Exeter, UK). Roberts said that the growing importance of carbocyclic nucleosides in antiviral therapy is exemplified by antiherpes agents such as cyclaridine and carbocyclic BVDU. Cyclopentane derivatives of this type often mimic the desirable biological activity of the corresponding (2'-deoxy) sugar, and moreover, show greater stability to enzyme-catalyzed degradation *in vivo*, according to Roberts.

The powerful antiherpes activity of the compounds FIAU and FMAU suggested to Roberts that the corresponding carbocyclic compounds might be of biological interest. The chemical synthesis of some of these compounds, as well as their biological activities as antiviral agents, was then presented by Roberts. In addition, he presented a new general method for the synthesis of carbocyclic nucleosides. This new route involves controlled intramolecular cyclizations of highly functionalized free radicals.

New purine derivatives with selective antiviral activity were discussed by M.R. Harnden (Beecham Pharmaceuticals Research Division, Biosciences Research Center, Great Burgh, UK). Harnden said that many

acyclic analogs of nucleosides have now been prepared, but only the N9-substituted guanines, acyclovir, ganciclovir, BRL 39123, buciclovir, and i-NDG have so far proved to be of major interest as selective antiherpes virus agents (see Figure 1). Harnden discussed the antiviral and biochemical properties of BRL 39123 and indicated the potential advantages in comparison with acyclovir. He

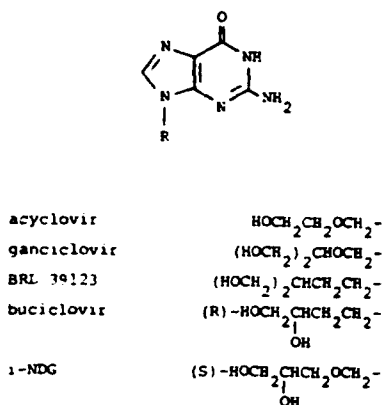


Figure 1. Selective antiherpes virus compounds.

also stated that this compound is now in clinical trials.

Harnden also reported on the synthesis of a novel series of N9-substituted purine derivatives via either imidazole or pyrimidine intermediates. Some of these compounds are also highly potent and selective inhibitors of herpes virus replication in cell culture. He compared their biological properties with those of the 9-hydroxyalkyl- and 9-hydroxyalkylmethyl-guanines.

Antibacterial, Antifungal, and Antiparasitic Agents

Fluconazole. Fluconazole, a novel systemically active antifungal agent was discussed by K. Richardson (Pfizer Central Research, Sandwich, UK). Fluconazole, a novel bis-triazole propanol derivative (see Figure 2), is the result of a research program at Pfizer aimed at discovering a broad-spectrum agent active by both oral and intravenous routes for the treatment of superficial and systemic fungal infections. According to Richardson, the imidazole/triazole series of antifungals were chosen as they are generally well tolerated, and triazoles were preferred to the usual imidazoles to minimize metabolic attack. Attention was then focused on polar derivatives in order to achieve high, sustained blood levels of un-

bound drug, and thereby maximize antifungal efficacy. This generated a series of 1,3-bis-triazole propan-2-ol derivatives with a wide range of substituents at the 2-position. The compounds were examined for efficacy against systemic candidosis, dermatophytosis, and vaginal candidosis in normal mice, and against systemic candidosis in immune-suppressed mice. The 2,4-difluorophenyl analog, Fluconazole, was chosen for development on the basis of potent antifungal activity, a long plasma half-life, high urinary recovery, and the ready achievement of an intravenous formulation due to its water solubility.

Evaluation in man has shown that Fluconazole is 100 percent absorbed orally, has a long half-life and is excreted unchanged in the urine. In vaginal candidosis a single dose is highly effective, according to Richardson, while good efficacy has also been seen with dermatophytosis. Fluconazole has now progressed into evaluation against systemic infections in leukemia, cancer, and AIDS patients, and the results are highly encouraging, according to Richardson. Also Fluconazole has been found to be very effective against *Candida* infections in the mouth, gut, throat, and kidney and against *Cryptococcus* infections in the brain. Richardson also said that early results are promising against systemic infections due to *Coccidioides*, *Blastomyces*, and *Histoplasma* infections. Thus, according to Richardson, Fluconazole is a drug that can be given once a day, either orally or intravenously, is highly effective against a broad range of fungal infections, and is active in both immune-normal and immune-compromised patients.

Antimalarial Hydroxynaphthoquinones. This subject was discussed by A.T. Hudson (Wellcome Research Laboratories, Beckenham, UK). Structure-activity studies on 2-cyclohexyl-3-hydroxy 1,4-naphthoquinones were carried out *in vitro* against one of the causative agents of malaria in man – i.e., *Plasmodium falciparum* – by Hudson and his group. They found that the t-butyl analog (called BW58C) had outstanding activity in the assay system, being effective at much lower doses than the currently used drug, chloroquinone. Evaluation *in vivo* against a variety of mammalian and avian *Plasmodium*

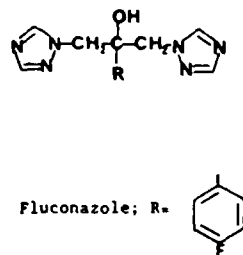


Figure 2. Fluconazole, an antifungal compound.

species showed comparable (or greater) efficacy than chloroquinone. However, although Phase I clinical trials on BW58C showed that it was well tolerated by healthy volunteers, it was extensively metabolized to the alcohol and other derivatives which had longer half lives than the parent compound. Therefore, further clinical evaluation was abandoned. Hudson and his group then carried out *in vitro* studies using hepatic microsomes from various species and other hydroxynaphthoquinones which had shown promising activity in the *P. falciparum* screening. Several compounds were found to have greater resistance to metabolism than BW58C. For example, the compound shown in (2) of Figure 3 was inert to microsome preparations from human, monkeys, and mice and was considerably more active than BW58C against *Plasmodia* in various animal models. Hudson thinks that the results are promising for obtaining a hydroxynaphthoquinone with sufficient metabolic stability and intrinsic activity against *P. falciparum* to be clinically effective.

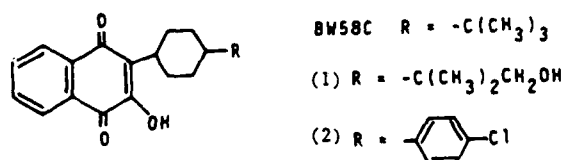


Figure 3. Antimalarial compounds.

Synthesis of Antibacterial Compounds. Approaches to the synthesis of antibacterial compounds were reported by E.J. Thomas (Dyson Perrins Laboratory, Oxford University). Thomas spoke about the development of an asymmetric synthesis of thiotetronic acids as well as synthetic approaches to milbemycins and avermectins – in particular, the synthesis of spiroacetal fragments of these compounds.

The chemistry of thiotetronic acids has been studied intermittently since Benary first studied the parent system (1), Figure 4. However, interest in this area has recently increased because of the isolation and characterization of several thiotetronic acid antibiotics including thiolactomycin (2), thiotetromycin (3), and U-68,204 (4) – all shown in Figure 4. Although a synthesis of racemic thiolactomycin has been reported, according to Thomas, no asymmetric synthesis of a chiral thiotetronic acid has been reported to date. However, Thomas and his group have been able to carry out the asymmetric synthesis of thiotetronic acids as represented by the thiolactomycin analogs (5 to 7), Figure 4. The key step in this work is the introduction of the chiral center at C(5) *vis* the highly stereoselective rearrangement of an allylic xanthate.

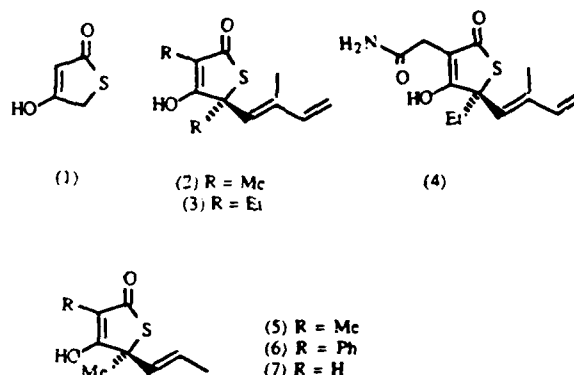


Figure 4. Thiotetronic acid antibiotics.

Thomas also discussed an approach to the synthesis of nonaromatic β -milbemycins, for example, milbemycin E, (1) Figure 5, which is based on a stereoselective Robinson annelation-furan oxidation strategy. A procedure for the regio-selective incorporation of the C(3)-C(4) double bond was reported together with asymmetric synthesis of the 'upper hemisphere' (3), Figure 5. Finally, Thomas outlined a concise asymmetric synthesis of the avermectin spiroacetal (4), Figure 5.

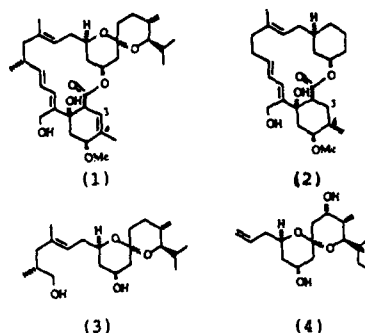


Figure 5. Nonaromatic milbemycins.

Application of Computing to Medicinal Chemistry

Use of X-ray and Computer Graphics. X-ray and computer graphics studies of renin-inhibitor aspartic proteinase complexes were reported by T.L. Blundell (Laboratory of Molecular Biology, Department of Crystallography, Birbeck College, University of London, UK). Inhibitors of the conversion of angiotensin II have considerable value as antihypertensive agents. For example, captopril and enalapril are clinically useful as inhibitors

of angiotensin converting enzyme (ACE). This has encouraged intense activity in the development of inhibitors of kidney renin, which is a very specific aspartic proteinase catalyzing the first and rate-limiting step in the conversion of angiotensinogen into angiotensin II. The most effective inhibitors such as H-142, H-261, and L-363,564 have utilized nonhydrolyzable analogs of the proposed transition state such as $-\text{CH}_2\text{NH}-$, $-\text{CHOH}-\text{CH}_2-$, or statine and partial sequences of angiotensinogen. H-142 is effective in lowering blood pressure in humans but has no significant effect on other aspartic proteinases such as pepsin in the body. According to Blundell there are no crystal structures available at present for human or mouse renins although three-dimensional models demonstrate close structural homology with other aspartic proteinases. Therefore, Blundell and his group have determined by x-ray analysis, the three-dimensional structures of H-142, H-261, BW-624, and L-363,564 complexed with the aspartic proteinase, endothiapepsin, which binds these inhibitors with affinities not greatly different from those measured against human renin. The structures of these complexes and that with the general aspartic proteinase inhibitor, H-256, define the common hydrogen bonding schemes that allow subtle differences in sidechain orientations and in the position of the transition state analogs with respect to the active site aspartates.

Blundell said that the x-ray studies define possible conformations of bound inhibitors which are likely to be relevant to the homologous enzyme, human renin. They provide the basis for detailed modeling to test this hypothesis, and, as a result of a better complementarity of shape, charge, and hydrophobicity in all the subsites, may also provide clues for the synthesis of analogs which are effective inhibitors of human renin. Blundell also indicated that intramolecular cyclization to increase rigidity and stabilize the bound conformation of the transition state analogs should also improve their effectiveness.

Use of Molecular Dynamics. The application of molecular dynamics in the prediction of accessible conformations was discussed by D.J. Osguthorpe (Molecular Graphics Unit, University of Bath, UK). Osguthorpe said that the use of theoretical chemistry techniques as an aid to drug design is rapidly becoming an integral part of any drug development program. The current interest of Osguthorpe and his group is the application of the technique of molecular dynamics in the drug design field, particularly in the area of peptide hormones and in receptor-based drug design.

According to Osguthorpe, there is currently much interest in the pharmaceutical industry in designing drugs by mimicking the peptide hormone controlling the faulty or diseased biological mechanism. Since these hormones

are highly flexible, an integral and major part of designing the drug is to find out what is the "active conformation" of the hormone. Osguthorpe and his group have applied this idea to the peptide hormone, Melanin Concentrating Hormone (MCH). They found that the hormone underwent significant conformational changes during a 150-picosecond simulation. Energy minimization of selected transient structures was carried out to reveal the equilibrium conformations underlying the dynamic motions. To evaluate the merits of this method of searching for active conformation(s), these investigators compared the results to a complete geometric search of the conformational space of the ring backbone.

Osguthorpe and his group are also using molecular dynamics as a tool for drug design when the structure of the receptor is unknown. In this field, the molecular dynamics simulation is used as an annealer and local minimum searcher. Using crystal structures of proteins that act as drug receptors, it is possible to attempt drug design by docking the new compounds in the experimental structure and examining the spatial fit and other interactions. However, Osguthorpe said, the formation of a drug-protein complex may be accompanied by significant conformational changes of the protein in addition to the drug. As energy minimization tends to stay in the initial local minimum, these investigators are using molecular dynamics to allow for larger conformational changes. They are also investigating conformational changes on ligand binding by distorting the protein along a low energy normal mode to accommodate the ligand. Osguthorpe and his group are applying these methods to ligands binding to Phospholipase A – in particular, to a modified substrate, a transition state analog, and the known inhibitor.

Conclusion

This focused and intensive conference on medicinal chemistry covered a broad range of topics, as indicated by this report. The presentations were given by scientists from academic institutions as well from industrial organizations. It is evident that the latter, especially pharmaceutical companies, are actively engaged in basic as well as applied research in the search for new and more effective drugs. The development of new drugs involves a multidisciplinary approach utilizing the expertise of scientists from many different backgrounds such as microbiology, pharmacology, biochemistry, organic chemistry, and molecular biology. Computer graphics and molecular dynamics are also playing an increasingly important role in drug design.

1/30/88

Biotechnology Conference

Extremophiles: Exploration and Exploitation

Claire E. Zomzely-Neurath.

Introduction

The European Federation of Biotechnology Working Party on Microbial Physiology arranged the Third International Symposium in the series titled "Microbial Physiology for Biotechnological Innovation." The theme chosen for the 1987 symposium was: Extremophiles: Exploration and Exploitation. The symposium, sponsored by the Society of Chemical Industry (Biotechnology Group) in collaboration with the Society for General Microbiology, took place on 3 and 4 December 1987 at the premises of the Society of Chemical Industry in London, UK.

There were 125 attendees at this focused conference with 68 percent from academic institutions and the remainder representing industrial organizations. Although the majority of delegates were from the UK, 15 West European countries were represented as well as the US, Canada, Israel, and East Germany.

It seems appropriate at this point to define "extremophiles." These are microorganisms which grow in naturally occurring extreme conditions of either acids, alkali, salt concentrations, high temperature, high pressures, or even on unusual carbon compounds. Such microorganisms may have a large potential for commercial development. Thus, an understanding of this potential and the fundamental physiology of the microorganisms was the subject of this symposium.

The scientific program consisted of a series of invited lectures by prominent researchers covering the various fields of the extremophiles; it also included 30 poster presentations. A summary of selected lectures and poster presentations is given in this report. There will not be any publication of the symposium proceedings.

Bacteria from Alkaline and Saline Environments

W. D. Grant (Department of Microbiology, University of Leicester, UK) discussed this topic. He said that stable, naturally-occurring highly alkaline environments ($> \text{pH } 10$) are uncommon due to the buffering effect of atmospheric carbon dioxide (CO_2). The most significant of such environments are the soda lakes characterized by the presence of large amounts of sodium carbonate and sodium chloride formed by extreme evaporative concentrations in arid areas of the world where the rocks lack

significant amounts of calcium and magnesium (which would remove CO_2 as insoluble salts). Soda lakes, although extremely alkaline ($\text{pH } 10\text{--}11.5$) and salty (up to 33 percent w/v $\text{Na}_2\text{CO}_3 + \text{NaCl}$) nevertheless harbor large populations of prokaryotes ranging from alkaliphilic cyanobacteria such as *Spirulina platensis* in the more dilute lakes to halokaliphilic archaeobacteria of the genera *Natronobacterium* and *Natronococcus* in the most concentrated lakes. Bacteria from such environments must have extremely efficient uptake systems for Mg^{2+} and Ca^{2+} (which are undetectable in such brines) and require energy-generating systems capable of functioning under conditions where the transmembrane pH gradient is reversed, according to Grant.

The halophilic archaeobacteria, Grant said, comprise two distinct halobacterial lines within the halophilic archaeobacteria. These prokaryotes require high pH, have asymmetric archaeobacterial ether lipids, and lack bacteriorhodopsin, although otherwise are clearly halobacteria. Such bacteria promote crystallization of salt in brines and become incorporated into fluid inclusions within crystals. Grant and coworkers found that within such inclusions, under presumed starvation conditions these bacteria remain viable for many years. Grant and his group found that halokaliphilic DNA can be readily cloned using cosmid systems—i.e., recombinant DNA methods—and in common with other archaeobacterial DNA's have AT-rich promoter-like sequences. Grant and his group are carrying out detailed characterization of these bacteria with the aim of their potential use in various biotechnological processes.

Metal Leaching by Acidophilic Bacteria

The contribution of iron- and sulphur-oxidizing bacteria to the extraction of metals, particularly copper, in leach dump systems has been recognized for over 20 years, according to P. Norris (Department of Biotechnology, University of Warwick, UK). Currently, where the geology is appropriate, there are some examples of the exploitation of this bacterial activity in slightly more technically developed systems.

According to Norris, underground bacterial leaching of fragmented ore in a Canadian mine is producing 70,000 pounds of uranium oxide per month; bacterial activity in thin-layer leaching on prepared surfaces is used in Chile to increase the copper extraction from sulphides follow-

ing acid dissolution of oxides; and in probably the most rapidly developing area of biohydrometallurgy, pilot plants are operating successfully for the extraction of gold from refractory sulphides.

Norris stated that the optimization and improvement of the bacterial activity has to consider a combination of extreme conditions comprising high acidity, low (in some regions) or high temperatures and high concentrations of toxic metals, including copper, uranium, and arsenic. Progress in recent years has been made in relation to the temperature with the description of apparently cold-tolerant strains of *Thiobacillus ferrooxidans* and of a range of thermophilic mineral-oxidizing acidophiles which can tolerate the heat generated by exothermic mineral oxidations and can degrade some minerals at rates several times faster than those associated with the mesophile *T. ferrooxidans*.

According to Norris, relatively little is known of the physiology of any of the acidophilic iron oxidizing bacteria apart from *T. ferrooxidans*. However, recent studies have indicated a variety of iron oxidation systems in different organisms; different responses of various acidophiles to particular toxic metals; and significant differences between organisms in their affinity for iron which, in the case of *T. ferrooxidans* and *Leptospirillum ferrooxidans*, for example, are sufficient for the latter to oust the former from initially mixed cultures of the organisms in iron-limited chemostats.

Norris stated that the study of the physiological characteristics of the various mineral-oxidizing bacteria which now can be considered as potentially useful for commercial processes is providing a clearer understanding of the observed patterns of mineral dissolution and a basis for more enlightened organism selection and process optimization.

Enteric Bacteria and Osmotic Stress

This topic was addressed by I. R. Booth (Department of Genetics and Microbiology, University of Aberdeen, UK). Booth said that the regulation of turgor (the pressure exerted by the cytoplasm against the cytoplasmic membrane) is essential for the growth of bacteria. The enteric bacteria, according to Booth, have evolved an impressive array of mechanisms that allow the cell to grow rapidly at different external osmotic pressures. The cells adjust their internal osmolarity to progressively higher values to maintain a relatively constant turgor pressure. The primary mechanism of turgor regulation, according to Booth, is the controlled accumulation of potassium and its counterion, glutamate. However, at high external osmolarities, the change in cytoplasmic ionic strength is inimicable to enzyme function, and thus cells grow slowly despite restoration of turgor. To counter the toxic effects of potassium, enteric bacteria have evolved the capacity

both to synthesize and/or to transport compatible solutes such as betaine (N-methylglycine), proline, and trehalose. Booth said that the accumulation of these solutes reflects the controlled functioning of transport and enzyme systems in response to changes in external osmotic pressure.

In their studies of enteric bacteria, Booth and his group have found that the bacteria's control over the balance of cytoplasmic osmolytes is achieved by sensing of the intracellular potassium concentration.

Environmental Microbial Degradations at Low Temperatures

Biological processes play an important role in connection with environmental pollution. Microorganisms naturally respond in discharge situations by enhanced growth of species able to utilize the pollutants. Furthermore, biological treatment processes are commonly used to treat municipal and industrial wastes. In such cases, temperature and the type of organisms are important for the efficiency of the biodegradation. Low temperatures have generally been considered a problem in such connections.

Studies have been carried out on low-temperature biological treatment of municipal wastewater in laboratory-scale experiments by G. Halmo (Department of Microbiology, University of Trondheim, Norway). Both the carbon oxidation (activated sludge) nitrification and denitrification were covered in these studies. The efficiency of sludges enriched at 3° to 5°C were compared to sludges enriched at 20°C. Each step was studied separately as well as with others in various combinations of process design. Low temperature sludges were found to be very efficient even at 3°C. According to Halmo, they have favorable technical characteristics, and reasonable process parameters seemed to be obtainable in a treatment process based on organisms selected at low temperature. The microbial populations in the sludges have been partly characterized. Differences were found between high- and low-temperature sludges with respect to morphological forms, specific growth characteristics, and enzyme activities.

Halmo said that natural degradation in response to a chemical discharge into the environment has been frequently observed and reported. The studies Halmo and his group have conducted have dealt with oil spills and have included both degradation of oil on polluted shorelines as well as in composting processes of wastes from cleanup operations. Halmo stated that through manipulation with air and nutrient addition, the oil degradation has been greatly enhanced. Thus, according to Halmo, full-scale treatment experience has shown that biodegradation is a relevant option for treatment even in cold climate zones.

Microalgae

Environmental stress as a tool in the exploitation of microalgae was addressed by Z. Dubinsky (Department of Life Sciences, Bar-Ilan University, Ramat-Gan, Israel). Microalgae, according to him, are very attractive organisms for biotechnological applications because they are naturally adapted for growth in liquid media under controlled conditions. Since they have no photosynthesizing tissues their potential light energy utilization is very high. Furthermore, these organisms respond to change in temperature, salinity, irradiance level, nutrient supply, and senescence by undergoing dramatic changes in their chemical composition. Dubinsky and his group have studied ways to utilize this biochemical plasticity in order to control growth rates and yields of lipids, polyunsaturated fatty acids (PUFA), and natural antioxidants. These researchers have studied a number of microalgae from various environments representing different taxonomic groups and have obtained economically interesting levels of PUFA and water-soluble antioxidants.

Thermostable Enzymes for Biotechnology

An overview of this topic was presented by T.K. Sundaram (Department of Biochemistry and Applied Molecular Biology, University of Manchester, UK). Sundaram said that a greater appreciation of the potential of enzymes for practical exploitation is part of the current surge of activity in biotechnology. Recent scientific advances which provide the means for a more efficient production and use of enzymes and the availability of thermophilic microorganisms as a source of enzymes stable at high temperatures are important developments in this area.

A relatively small number of enzymes account for the market for industrial enzymes worth about \$500 million. A majority of these enzymes are extracellular hydrolases such as proteinases and carbohydrases (a notable exception being xylose isomerase, used in the production of high-fructose corn syrup). Enzyme-catalyzed industrial reactions are run at relatively high temperatures (50°C or higher). According to Sundaram, several advantages accrue from the high-temperature operation of enzymic industrial processes; for example: (1) higher reaction rates resulting from kinetic effects, reduced viscosity and surface tension, and increased solubility and diffusion of reactants; (2) maintenance in liquid state of reactants with high melting points such as fats in triglyceride modifications; (3) lower risk of microbial contamination; and (4) sometimes a desirable shift in reaction equilibrium. Sundaram said that the greater storage stability of thermostable enzymes will also contribute to savings in costs. Thermostable enzymes are generally also more resistant to chemical denaturants; this property makes

them suitable as catalysts for the synthesis of organic chemicals and for reactions which entail the use of organic solvents. According to Sundaram, the availability of the required thermostable enzymes at an economic cost therefore becomes an important factor in enzymic industrial processes. Most of the industrial enzymes are currently derived from a comparatively small number (about 25) of microorganisms.

Although enzymes from thermophiles are invariably more thermostable than their mesophilic counterparts, thermophilic organisms are not used extensively as a source of industrial enzymes. According to Sundaram, most of the thermostable industrial enzymes come from mesophiles, a notable example being the α -amylase of *Bacillus licheniformis*, which is used at 90° to 110° C for liquefying starch. Some of the reasons for this situation are the following. The cultivation of thermophiles with high optimum growth temperatures can present problems, as indicated by the experience with *Thermus*, which otherwise is a good source of thermostable enzymes. Also, genetic instability and strain variability have been reported with extreme thermophiles. Enzymes from thermophiles are, in general, less active at moderate temperatures than those from mesophiles, but at the higher temperatures at which they can function, their activity will match that of the mesophilic enzymes at the moderate temperatures. Therefore, unless the reaction conditions can exploit this facility of thermophilic enzymes, there may be little advantage in using them in industrial processes. Despite their greater inherent stability vis-a-vis their mesophilic counterparts, thermophilic enzymes may still need to be stabilized during industrial use and this, according to Sundaram, may pose problems.

Notwithstanding the above considerations, the potential of the intrinsically more stable thermophilic enzymes is well recognized. Most of the work on thermophilic enzymes has been done with organisms from only two genera, *Bacillus* and *Thermus*. According to Sundaram, a recent encouraging development is the discovery of thermophiles outside these genera. Of particular interest are the archaebacteria growing optimally at 80° to 105°C, of which some are acidophiles. This extends the range of thermophiles available for exploitation. However, a great deal of basic research and development is needed. Genetic engineering should play an important role here. For example, mesophilic organisms carrying clones of thermophile genes could serve as satisfactory sources of thermophilic enzymes. Another approach is to develop cloning systems in thermophilic organisms. Protein engineering holds forth the prospect of altering enzyme activity and stability to suit particular needs. There are also other, less glamorous ways to alter enzyme stability—chemical modification, for example, and immobilization. Sundaram said that research is under way

on several of these aspects. The translation of the potential of the thermostable enzymes of thermophiles into a realistic niche in biotechnology appears likely to depend on whether further research can solve the problems mentioned above and make the production and use of these enzymes economically viable.

Hyperthermophilic Bacteria. Hyperthermophilic bacteria growing optimally above 80°C have been isolated from acidic and neutral solfatara fields and submarine hydrothermal systems by K.O. Stetter (Institute for Microbiology, University of Regensburg, West Germany) (Stetter, 1986). The most extreme hyperthermophiles are members of the genera *Pyrodictum*, *Pyrococcus*, and *Pyrobaculum*, growing optimally at above 100°C under slight overpressure. Hyperthermophiles are aerobic, facultatively anaerobic, and, in most cases, obligately anaerobic organisms belonging almost exclusively (with the exception of *Thermotoga*) to the archaeobacteria. They are chemolithoautotrophs and heterotrophs. Hyperthermophiles occur within both phylogenetic branches of archaeobacteria. Stetter said that the few enzymes from these organisms which have been studied *in vitro* show a different heat sensitivity. Stetter thinks that it most likely parallels the phylogenetic position of the organism rather than its maximal growth temperature.

Bicalorimetric Studies of Thermophilic Microorganisms. A device for isothermal heat measurement during microbial processes was described by B. Heinritz (Institute of Biotechnology of the Academy of Science of the German Democratic Republic, Leipzig, East Germany). On the basis of calorimetric measurements using their device, Heinritz and coworkers determined the dependence of specific heat production of thermophilic bacteria, especially *Bacillus* species, on reaction conditions. They found that the specific heat production and carbon substrate conversion of thermophilic microorganisms was higher than values for mesophiles. Heinritz said that this finding could be explained by the increased energy dissipation of microorganisms for maintenance of cell structures under extreme physicochemical conditions. The oxycaloric coefficient of carbon substrate conversion by thermophiles was found to be close to the theoretical values under the experimental conditions used by Heinritz and his group.

Metabolism of Carbamoylphosphate in Extreme Thermophilic Bacteria. The metabolism of carbamoylphosphate, a highly thermolabile precursor of arginine and pyrimidine biosynthesis, was studied in two extreme thermophilic organisms, *Thermus aquaticus* (eubacterium) and *Sulfolobus solfataricus* (archaebacterium), by C. Legrain (Research Institute of Food and Chemicals, Free University of Brussels, Belgium). Legrain and his group found that the carbamoylphosphate synthetase and the aspartate carbamoyltransferase of *T. aquaticus* were quite similar to their mesophilic counterparts with

respect to their size and kinetic properties, but were stable at temperatures up to 90°C. Both enzymes were found to be feedback-inhibited by pyrimidine nucleotides, raising the problem of allosteric control at high temperature.

Legrain and coworkers found that the ornithine carbamoyltransferase of *T. aquaticus* is reversibly inactivated by a "cryoscopic shock," which suggests a temperature-mediated conformational change, according to Legrain. The carbamoyltransferases of *Sulfolobus* were found to be devoid of regulatory properties. Their molecular weights are considerably higher than those of *T. aquaticus* or of the mesophilic transferases, possibly indicating a different strategy for resistance to elevated temperature.

Comparative Studies of Amino Acid Dehydrogenases from Mesophilic and Thermophilic *Bacillus* Strains. These studies were carried out by U. Kärst (Institute for Biotechnology, Braunschweig, West Germany). Kärst said that the genus *Bacillus* comprises mesophilic, moderately and extremely thermophilic, and thermoacidophilic species. This has the advantage of permitting the comparison of enzymes optimized for very different conditions of life from within a quite homogeneous and closely related group of microorganisms.

Kärst and his group had previously purified and characterized a leucine dehydrogenase (LeuDH) from the mesophilic *B. cereus* which had already been tested as a catalyst for the biotechnological production of L-leucine, L-methionine, and L-tert-leucine. In order to improve the stability of this LeuDH by protein engineering techniques, Kärst and his group screened thermophilic *Bacillus* strains for a heat-stable phylogenetically related counterpart to the mesophilic enzyme using antibodies against this LeuDH as a probe.

Ten of the 16 strains examined (which were obtained from the German Center for Microorganisms, Göttingen, West Germany) showed a strong cross-reaction of the partial identity type. Kärst and his coworkers selected the extremely thermophilic *B. caldolyticus* (DSM 405) as the most appropriate strain. These researchers purified and characterized the LeuDH and alanine dehydrogenase (AlaDH) from this organism and compared their physical and biochemical properties with those of the respective enzymes from *B. cereus*.

The comparison of thermophilic versus mesophilic for each enzyme pair revealed a high degree of similarity. The molecular weights, the mass, and number of subunits of both enzyme types and the quaternary structure in the case of the LeuDH's were found to be almost identical. However, the isoelectric points of the enzymes differed by 0.8 and 0.5 pH units for the LeuDH's and AlaDH's, respectively, with the mesophilic enzymes being more acidic. Furthermore, pH-stability, pH-optima, stability in aqueous solution, K_m values for coenzymes and sub-

strates, and the pattern of inhibition by different compounds such as sulfhydryl reagents and pyridoxal-5-phosphate in the case of the LeuDH's, were also similar. Kärst said that this also applies to the amino acid composition and the N-terminal amino acid sequences of the LeuDH's, indicating that the genes encoding them evolved from a common ancestor. Thus, Kärst and his group found that the only major difference between the mesophilic and thermophilic enzymes was the much higher stability of the latter against denaturation by heat and organic solvents. Kärst said that these properties make the thermophilic enzymes very suitable and attractive as industrial biocatalysts and for protein engineering studies regarding the evaluation of those structural features that confer the increased stability.

Study of Secondary Transport Processes in Thermophilic Bacteria. W.N. Konings (Department of Microbiology, University of Groningen, the Netherlands) described a study of primary transport systems as a useful tool for investigating secondary transport processes in thermophilic bacteria. Enzymes from thermophilic organisms share as a common property their extreme thermostability. Konings said that from this point of view, it seems obvious that, in particular, enzymes of these organisms offer nice model-systems and are extremely well suited for large-scale purification and biochemical characterization.

Konings and his group attempted to characterize solute (sugars and amino acid transport) processes which are located in the cytoplasmic membrane of the moderate thermophile *B. stearothermophilus*. The solute transport (secondary transport) can be studied in isolated cytoplasmic membranes from this organism but due to the presence of respiratory chain components and other secondary transport processes, interferences can be expected, according to Konings. He said that mechanistic studies of a specific transport process would be considerably improved by using a purified transport system incorporated into artificial membranes. However, in order to study active solute transport in artificial membranes, electrochemical energy (proton-motive force) is required as a driving force. Because of the high temperature optima of the transport processes in thermophilic organisms, one needs, Konings said, to incorporate a proton-motive force generating system capable of functioning at high temperatures in order to study these processes in reconstituted systems.

Therefore, Konings and his group isolated a proton-motive generating system from the thermophile *B. stearothermophilus*. The terminal component of the respiratory chain, a *caa3*-type cytochrome *c*-oxidase is capable of converting redox-energy into electrochemical energy. By means of selective solubilization and ion-exchange chromatography, this component was purified

and reconstituted into artificial membranes by Konings and coworkers. The enzyme is capable of a high rate of oxidizing of cytochrome *c* from different origins and also of artificial electron donors. The reconstituted enzyme generates a high proton-motive force, consisting of an electrical potential and a pH-gradient, across the artificial membrane. Due to its high stability over a wide range of temperatures, it is very suitable for the study of the mechanistic aspects of reconstituted solute transport from thermophilic organisms in these model systems, according to Konings.

Regulation of Methanol Metabolism in Thermotolerant Bacilli. A.G. Brooke (Department of Microbiology, University of Sheffield, UK), who reported the study on this subject, said that an enormous diversity of microorganisms is able to grow on methanol, a compound of relatively low cost and increasing worldwide production which therefore is attractive as a raw material for biotechnological processes. However, of the aerobic methylotrophic bacteria so far isolated, the vast majority have been Gram-negative mesophiles which, in general, appeared sensitive to concentrations of methanol in excess of 100 mM. Recently, using newly developed techniques, a number of thermotolerant (temperature optimum of 50° to 52.5°C) methylotrophic spore-forming bacilli have been isolated by Brooke and his group as well as by some researchers in the Netherlands. These organisms have been found to tolerate methanol concentrations up to 1.5 M. Hence, according to Brooke, these bacilli might be expected to possess considerable industrial potential, not only as synthesizers of thermotolerant (perhaps novel) enzymes, but also for the transformation of methanol to useful low-molecular-weight metabolites.

According to Brooke, in order to assess the utility of these organisms for biotechnological processes it is necessary first to understand more of their basic physiology and biochemistry. In particular, it is important to determine the pathways of methanol utilization, the mechanisms of regulation of methanol metabolism, and the extent to which methanol catabolism can be dissociated from anabolism. Brooke said that from such studies one might better assess the potential of these organisms to produce compounds of industrial interest, or reveal targets for genetic manipulation that would allow methanol metabolism to be steered to the overproduction of desired products. Work along these lines by Brooke and his group is now in progress, and he presented preliminary data.

A Novel Archaeobacterial Alcohol Dehydrogenase. A report on the structure and properties of a novel archaeobacterial NAD⁺-dependent alcohol dehydrogenase was presented by M. Rossi (Department of Organic and Biological Chemistry, University of Naples, Italy). Rossi said that alcohol dehydrogenase (ADH) isolated from

different sources shows different substrate specificities. Yeast enzyme can catalyze oxidation of primary and secondary alcohols while horse liver ADH exhibits a broad specificity and catalyzes even the oxidation of cyclic alcohols such as cyclohexanol. However, the wide biotechnological applications in stereospecific organic synthesis and in the production of high-value added products has been limited by the low stability to organic solvents of different enzymes, according to Rossi. Thus, Rossi and his group have focused on enzymes from extreme thermophilic archaeobacteria. Many enzymes isolated from these organisms have been found to be thermostable and capable of acting at high temperature. In addition, they show a general stability to the common protein denaturants, such as sodium dodecyl sulfate, urea, and organic solvents.

Rossi and coworkers purified a novel alcohol dehydrogenase (Rella et al., 1987) to homogeneity from the archaeobacterium *Sulfolobus solfataricus* (SsADH). The subunit structure was studied by gel filtration, sucrose or gradient centrifugation, and electrophoresis in sodium dodecyl sulfate of the native protein and also crosslinked with dimethylsuberimidate (DMS). With these methods the enzyme was shown to be composed of two very similar or identical subunits of 37,000 daltons. The purified SsADH, which can be defined, according to Rossi, as an NAD^+ -linked alcohol aldehyde/ketone oxidoreductase, displayed activity towards aldehydes, a variety of primary and secondary alcohols as well as linear and cyclic ketones.

The apparent K_m values for different substrates were in the order of micromolar concentrations except for ketones like acetone, butanone and cyclopentanone. Rossi and his group found that the enzyme thermophilicity was quite extraordinary. In fact, the activity increased with temperatures up to 95°C, and the activation energy, calculated from the Arrhenius plot, was 47.8 kJ. SsADH displayed a considerable thermostability which was not influenced by the presence of certain organic solvents.

The stereospecificity of SsADH was tested on 3-methyl-butan-2-one. The reduction was performed on a gram scale with Eupergit C immobilized pure enzyme. NADH regeneration was achieved *in situ* with the coupled substrate approach, using propan-2-ol as oxidizable cosubstrate in 13-fold molar excess with respect to ketone. The number of NADH cycles obtained in the experiments was about 20,000 after 24 hours' reaction, when 50 percent of the ketone was converted into alcohol and 3.8 percent of propan-2-ol was oxidized to acetone. The enzyme is being assayed also in whole cells, and studies by Rossi and his group are now in progress on the asymmetric reduction of aliphatic ketones of different lengths and structures for comparison with the results obtained with purified or immobilized enzyme.

Glucose Dehydrogenase. A study of glucose dehydrogenase isolated from *Thermoplasma acidophilum* was reported by N. Budgen (Department of Biochemistry, University of Bath, UK). He said that the nicotinamide nucleotide-dependent dehydrogenases of eubacteria and eukaryotes are characteristically specific for either NAD^+ or NADP^+ and that it is uncommon to find such enzymes which are catalytically active with both cofactors. However, a number of dehydrogenases have now been extracted from the thermoacidophilic archaeobacteria which accept both NAD^+ and NADP^+ on the same protein molecule. According to Budgen, this dual cofactor-specificity, couple with extreme thermostability, renders these dehydrogenases of considerable biotechnological potential, as, for example, in NAD/NADP regeneration systems in organic synthesis.

Budgen and his group reported on the purification and properties of one such enzyme, glucose dehydrogenase, from *Thermoplasma acidophilum*. In addition to its thermostability and activity with both NAD^+ and NADP^+ , the enzyme was found to be remarkably stable to organic solvents and has the distinct advantage of oxidizing an inexpensive and readily available substrate.

Halobacteria

A report on the characterization of an extremely salt-tolerant marine bacterium was presented by D.J. Gilmour (Department of Microbiology, University of Sheffield, UK). Gilmour said that a rod-shaped bacterium was found to be a persistent contaminant of cultures of the unicellular halophilic green algae *Dunaliella* grown in media containing a wide range of sodium chloride concentrations. This bacterium was isolated by Gilmour and his group and found to have the following characteristics: (1) gram negative straight rods, motile by 6 to 8 peritrichous flagella; (2) chemoheterotrophic, obligate aerobic; (3) accumulates poly- β -hydroxybutyrate; (4) and is oxidase and catalase positive.

The bacterium is able to grow on a wide variety of carbon compounds including DL- α -alanine, proline, fumarate, glycerol, D,L- β -hydroxybutyrate, D,L-lactate, D,L-malate, succinate, and glucose. On the basis of these data, Gilmour has assigned this bacterium tentatively to the genus *Alcaligenes*.

Production of PHB and Polysaccharides by some Halobacteria. This topic was presented by F. Rodriguez-Valera (Department of Microbiology, University of Alicante, Spain). *Halobacterium mediterranei*, a species of halobacteria, has been recently described by Rodriguez-Valera and his group and has been found to produce large amounts of poly- β -hydroxybutyrate (PHB) and an extracellular polysaccharide when grown under adequate conditions. These researchers have studied the

parameters affecting the production of both polymers and also the composition and some properties of the polysaccharide. Rodrigues-Valera said that the singularity of the media required for growth of halobacteria drastically reduces the sterility precautions which would be needed for production of any of those compounds. The group is now exploring the possibility of growing these organisms in open cultures, and even in saltern ponds.

Conclusion

It is evident from the above report that many researchers in Europe and the UK are engaged in basic studies of bacteria which survive in extreme environments such as high salt, high pH, high temperature, etc. The recent interest in these types of organisms is the potential

for their use in biotechnological processes – in particular, the enzymes isolated from these Extremophiles. However, the studies are still at an early stage, and further work is necessary both in characterization of the enzymes as well as development of information on the physiology of these Extremophiles.

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3/13/88

Biotechnology Conference: Diagnostics '87

Claire E. Zornzely-Neurath

Introduction

The conference entitled "Diagnostics '87" was part of the Cambridge Series on Biotechnology organized by IBC Technical Services, London, UK. This focused and informative conference, planned by C.R. Lowe, University of Cambridge and C.P. Price, Addenbrookes's Hospital, Cambridge, UK, took place at the university's Churchill College on 10 and 11 December 1987.

There were 177 attendees at this conference, the majority from the UK. However, 11 European countries were also represented as well as the US, Australia, and India. Seventy-five percent of the participants were from industrial organizations with the balance from academia.

The conference program consisted of the following topics:

- Diagnostics – the impact of the new technologies
- Clinical diagnostics
- Reagent strip technology
- Thin-film technology
- Single-step immunoassay systems
- Enzyme-amplified immunoassays
- Fluorescent and luminescent immunoassay
- Rapid microbial assay technology
- Diagnostic applications of gene probe technology
- DNA probe technology – *in situ* hybridization assays
- New amperometric biosensors
- Application of electrochemical methods to immunoassays

- Magnetic resonance techniques in diagnostic medicine.

The last decade has seen dramatic improvements in the technologies underlying the development of diagnostic procedures. This progress is linked with the discovery of, and improvements in, conceptually new approaches such as amplified enzyme-linked immunoassay, strip and thin film technologies, fluorescence and luminescence immunoassay, DNA probe technology, and biosensors. The aim of the conference was to review the current status and likely developments in these new technologies, allow comparisons between competitive technologies, and assess their likely impact on the market for diagnostic products.

These new developments in diagnostic technologies are likely to have a profound effect on the way analytical procedures are performed, with a move away from specialized central facilities towards real-time analysis at the site of incidence. This trend will not be restricted to clinical diagnostics but may also apply to agricultural, horticultural, veterinary, pharmaceutical, and biotechnology-based analytical procedures. The conference was designed to address these implications and thus had appeal to research and technical personnel, product development, and marketing staff.

A summary of selected topics from this intensive and focused conference will be presented in this article. A more detailed survey is given in ONRL Report 8-006-C.

There are no plans for publication of the proceedings of this conference.

The Presentations

Diagnostics – The Impact of the New Technologies.

An overview of this topic was presented by G.T. Walker (Base International Limited, Milton Keynes, UK). Walker said that the fast growth in AIDS testing, and also the appearance of dry strip formats for the rapid identification of infectious organisms bears witness to the continued ability of novel technology to open up new market opportunities. The development of monoclonal antibody (Mab) technology over the past 10 years is already having an impact on diagnostic testing, together with complementary developments in nonisotopic labeling, according to Walker. Also, he said, improved antibodies for cancer monitoring are fuelling growth in that area at over 25 percent per year. Regionally, growth in these immunoassay applications is expected to be strongest in Western Europe, where a combination of receptivity of the market to automated technology and to a lower degree of market saturation than in the US is likely to make the whole market grow faster than anywhere else in the world. By 1990 it is expected that Western Europe will have grown to 38 percent of the world market, while North America will have declined to 35 percent.

Another growth area is that of tests suitable for the doctor's office. A site which has sustained growth over a long period is the home, in which monitoring tests for diabetics have predominated. Monoclonal antibody (Mab) technology, according to Walker, is already adding to growth in pregnancy tests, and with the recent launch of an amperometric biosensor into the diabetic glucose test market one can expect to see further impacts from this technology.

Walker also discussed evolving technology. He said that the forward view of immunoassay development is that sensitivities of nonisotopic labels will be further improved, together with the specificities of the antibodies, in order to carry out the applicability of the technique into areas which are currently only accessible via labor-intensive methods. In this way, growth in the diagnostic reagent market will be at the expense of cell-culture techniques or visual inspection of microscope slides and the like. A major technology for simplifying test procedures is the reagent strip, multimembrane structure, with which sample preparation and manipulation can be performed without the need for a skilled operator. The technology is already widely adopted for infectious organism testing, and it is expected that its use will be extended to other immunoassay applications, according to Walker.

Another evolving technology is the use of DNA probes. Several versions of this technology have emerged recently, seeking to simplify and to automate the skilled

task of gel electrophoresis and Southern blotting. DNA/RNA probe techniques are aimed at infectious microorganisms, at viruses, and at oncogenes. Thus, there is considerable overlap with Mab techniques. Since DNA probe technology is at a much earlier stage of development than Mab techniques, the major impact of this technology is not expected until after 1990, according to Walker.

Biosensors – sensors capable of mediating the concentration of an analyte directly into an electrical signal – have not yet made much impact on the clinical diagnostics market. Ion-specific electrodes have been developed for the analysis of electrolytes and blood gases as well as for glucose measurement. However, there is a new generation of biosensors, in which the use of immobilized enzymes, electron transfer mediators, and cheap methods of mass production should extend the use of biosensors first into a much wider range of metabolites, and later into immunoassay. Walker said that the number of research groups in the UK active in clinical biosensor development makes the UK a very exciting center in the world scene. There are also groups in the UK working on fiber optic and waveguide sensors.

Thin-Layer Technology. A report on thin-film technology was presented by J.F. Padday (Research Division, Kodak Limited, Wealdstone, Harrow, UK). This technology was developed in support of the EKTACHEM DIAGNOSTIC PROCESS originating at Kodak.

The properties of simple ions and molecules exhibit widely differing properties when adsorbed as monolayers according to whether the interface is solid/gas, solid/liquid, or liquid/gas. Macromolecules, polymers, or proteins adsorb in an entirely different way and tend to create the first stages of thin-film formation. The properties of adsorbed molecules and of thin layers were described by Padday as well as dynamic equilibria of both physical and chemical properties. According to Padday, when such properties are under control, it is then possible to use such properties for certain types of diagnostic procedures such as measurement of the amount of certain constituents of human body fluids, which are present in blood plasma, serum, and urine. Some examples are inorganic ions such as potassium, sodium, chloride, bicarbonate, etc.; triglycerides; creatinine; ammonia; and enzymes such as amylase, alkaline phosphatase, etc.

Reagent-Strip Technology. This topic was presented by W.E. Hornby (Research and Development Department, Unipath/Oxoid Limited, Bedford, UK). He said that the use of paper-based reagent strips for the rapid analysis of urinary constituents has been in common practice for many years. Recently, similar reagent-impregnated strips, developed for the measurement of glucose in whole blood, have made it possible for diabetics to monitor their blood glucose at home. The past decade has witnessed even further developments in reagent-strip

technology to the extent that these devices can now be used for measurement of a much wider range of analytes including drugs, enzymes, and components of immuno reactions. Hornby addressed these latest innovations, in particular those relating to rapid immunochemical test systems.

Clinical Diagnostics. In his overview of clinical diagnostics, C.P. Price (Addenbrooke's Hospital, Cambridge, UK) said that analytical tests on biological fluids can provide the clinician with vital information. A variety of analytical principles may be employed, foremost being enzyme- and antibody-mediated techniques. Tests may be required in a variety of circumstances – in the home, health care center, clinic, ambulance, ward, or operating theater. He said that the challenge in designing new diagnostic tests is to produce a system that provides sensitivity, specificity, simplicity, and speed of delivery appropriate to the clinical need.

Single-Step Immunoassay Systems. This topic was addressed by T.S. Baker (Department of Research and Development, Boots-Celltech Diagnostics Limited, Slough, UK). Baker said that the availability of new, simple to use, immunoassay technology is an important factor responsible for the emergence of the Alternate Site diagnostics market. He described a novel ImmunoStrip system which avoids all reagent additions/washings, has automatic reaction timing, and yields results within 10 minutes of sample collection. The ImmunoStrip system can incorporate both competitive and two-site immunoassays and has been demonstrated in tests for haptens, macromolecules and viral and bacterial samples.

Enzyme-Amplified Immunoassays. A. Johansson (Novo Biolabs, Cambridge, UK) spoke about the technique of enzyme-amplification, which is a method for enhancing the speed and sensitivity of enzyme immunoassays. Essentially the method uses the enzyme label as a "pre-amplifier" in order to increase greatly the apparent activity of the enzyme label itself. The enzyme-amplifier can produce either an intensely colored formazan dye, or can be coupled to an organic conducting salt or platinum electrode.

Fluorescent and Luminescent Immunoassay. In his presentation of this subject, J. Landon (Department of Chemical Pathology, St. Bartholomew's Hospital, London, UK) said that fluorescent and luminescent immunoassays can be designed to meet varied requirements. Nonseparation polarization fluoroimmunoassays currently dominate in areas where a quantitative result is required and sensitivity is not a problem such as in therapeutic drug monitoring, according to Landon. Alternatively, he said that several highly sensitive immunoassays based on chemiluminescence and time-resolved fluorescence promise to replace assays employing isotopically labeled antigens and antibodies.

Rapid Microbial Assay Technology. A. Swain (Biotechnology Center, Cranfield Institute of Biotechnology, UK) presented a survey of this topic as well as of the research carried out by him and his group. Swain said that rapid methods for the detection of microbial activity/contamination have received increasing attention in recent years for applications across the whole spectrum of biotechnologically based industries. He briefly reviewed the many alternative approaches available for the rapid detection of microbial biomass and described in detail a new mediated amperometric approach developed at the Cranfield Biotechnology Center. Swain described a prototype instrument based on this technology, the Biocheck, and presented results of its use showing the application of this technique to a wide range of microorganisms in a variety of relevant samples.

Gene Probe Technology. The diagnostic applications of gene probe technology were discussed by T.M. Twose (Department of Research and Development, ICI Diagnostics, Cheshire, UK). This method is still at an early stage of development as far as routine diagnostics is concerned, according to Twose. He said that its adoption is limited at present by the difficulty and complexity of the methodology. However, several clear strategies are emerging to circumvent the difficulties, and the particular advantages of gene probes are being increasingly successfully exploited to solve diagnostic problems. Twose outlined international developments and future prospects for this potentially valuable technology.

Magnetic Resonance Techniques in Diagnostic Medicine. This topic was discussed by L.D. Hall (Laboratory for Medicinal Chemistry, Addenbrooke's Hospital, University of Cambridge School of Clinical Medicine, UK). He said that the responses from magnetic nuclei in human tissues, such as protons in water and fat, provide the basis for a diverse family of noninvasive diagnostic procedures. So far, two members of this family have been most widely used: magnetic resonance imaging (MRI), which provides slice-images at any angle through the intact body that depict both anatomy and the location of pathology; and MR-spectroscopy, which gives a direct measure of the metabolic status of the tissues. Hall said that other methods can be used to map blood flow.

New Amperometric Biosensors. The concept of the exploitation of enzyme entrapment within conducting polymers in amperometric biosensors was presented by B. Yon Hin (Biotechnology Center, University of Cambridge, UK). This new enzyme immobilization procedure allows very precise control on the spatial distribution of the enzyme at the surface of the electrode, thus promoting proximity between enzyme and sensing electrode, according to Yon Hin. The technique has been applied by Yon Hin and his group to a microfabricated multielectrode device for use as an amperometric biosensor.

New Amperometric Biosensor Methods. This topic was addressed by P.N. Bartlett (Department of Chemistry, University of Warwick, UK). He said that a number of techniques have been developed over the past few years to enable amperometric electrodes to be linked electrochemically to redox enzymes and to thus produce biosensors. These methods include the use of novel electrode materials, modified electrodes, soluble redox mediators and enzymes modification. Bartlett discussed these methods and gave examples of their applications in biosensors.

Application of Electrochemical Methods to Immunoassays. The current trend away from radioimmunoassays has stimulated interest in the applications of electrochemical detection systems, according to M.J. Green (Research Department, Genetics International, UK). Many of these assays are more complex than existing colorimetric tests, he said. Some immunoassays have been designed which are merely adaptations of existing spectrophotometric assays while others have been designed with suitable electrochemical signals. Green discussed the merits of some of these system in his presentation.

DNA Probe Technology – *In Situ* Hybridization Assays. A rapid nonradioactive *in situ* DNA probe assay for detecting human papilloma viruses (HPV) in ano-genital biopsy specimens was described by N. Kelker (Enzo

Biochem, Inc., New York). He said that this test can be used to identify specific HPV types and to predict the likelihood for developing HPV-related cancer. Kelker also discussed the application of this technology to the detection of other pathogens.

Conclusion

Most of the presentations in this conference on diagnostic procedures were given by scientists from industrial concerns. Thus, many such organizations are heavily engaged in research and development of diagnostic methods. This is not surprising since the area of diagnostic methods is at present a sizeable market and has tremendous potential for the future. It is also evident from the above brief summaries that UK companies as well as UK branches of US companies are making important contributions to the development of more sensitive and simplified diagnostic tests. The topic of biosensors received considerable attention as, again, the potential market is extremely large once the problems encountered with the practical use of biosensors have been worked out. At present the UK is dominant in biosensor research, particularly at the Biotechnology Centers in Cambridge and Cranfield.

2/13/88

CHEMISTRY

International Society of Electrochemistry Meeting

by Kurt H. Stern. Dr. Stern is a research scientist in Surface Chemistry, Chemistry Division, Naval Research Laboratory, Washington,

The International Society of Electrochemistry held its 38th meeting in Maastricht, the Netherlands, from 13 through 18 September 1987. This organization has been in existence since 1970 and its annual meeting, held in a different country each year, serves as a gathering for European electrochemists—academic and industrial—with some attendance by US, Japanese, and Latin American scientist.

This year's meeting, with its theme of "Electrochemistry for New Materials and New Materials for Electrochemistry," attracted approximately 500 attendees, most of whom presented posters—70 or so each day. Five plenary lectures were presented (one a day) and 18 keynote lectures (two simultaneous ones in the

mornings and afternoons). Following is a brief summary of selected papers.

Two Overview Lectures

The meeting began with the presentation of the Debye (Debye in Dutch) lecture by Heinz Gerischer (Fritz Haber Institute, West Berlin), who first presented a detailed biography of Peter Debye, Maastricht's most distinguished scientific son. In the remainder of his lecture Gerischer reviewed the interactions of light with metal and semiconductor films, and how electrochemical measurements can contribute to probing these interactions. The physical principles are, of course, very ap-

of the Fritz Haber Institute, who described the techniques currently used in this field. *In situ* reflectance spectroscopy in the IR through UV range, and even x-rays have been employed to reveal surface symmetries and electronic surfaces under potential control. *Ex-situ* methods, such as low-energy electron diffraction (LEED), are used to probe changes on surface structure after electrochemical treatment by transferring the electrode from the solution into ultrahigh vacuum without exposing it to the atmosphere.

Measuring Electrical Events

The first 2 days of the conference were devoted to various aspects of the central concern of electrochemistry: how to measure and control events occurring on the electrode surface and in the adjacent solution region (electrical double layer). Increasing sophistication in the purely electrochemical aspects of such measurements was exemplified in the paper by M. Sluyters-Rehbach (University of Utrecht, the Netherlands) who discussed the analysis of charge transfer in catalysis and inhibition, and his group's use of high-precision impedance voltammetry in probing the kinetics of individual electron transfers in multistep (multi-electron) reactions.

A complementary approach, the combination of electromagnetic and electrochemical measurements to probe surface states when the material is under electrochemical control, as exemplified by the talks of Gerischer and Kolb, has already been mentioned. It has long been realized that the standard materials, mainly metals, are not sufficient to provide the selectivity and catalytic activity which is desired in electrochemical reactions, e.g., how to make only a single product. For the past several years this concern has been addressed by modifying the electrode surface. E. Barendrecht (University of Eindhoven, the Netherlands) described two kinds of modifications: physical modification, in which the porosity and roughness of the electrode is changed; and chemical modification, in which molecules, sometimes long chain compounds are anchored to the electrode surface, so that a new surface is, in effect, created. These materials may be attached by adsorption, covalent binding, or polymer film formation. R.W. Murray (University of North Carolina, Chapel Hill) discussed in greater detail the attachment of very thin polymer films on electrodes and the measurement of electron transport through them. His group has pioneered the development of very thin sandwich electrodes (solid-electrode/polymer-film/porous-electrode) with the polymer thickness in the 50- to 200-nm range. The advantage of this thin film is that electron exchange through the polymer can be accomplished on observable time scales, and steady-state currents can be measured for

events on both sides of the film as well as electron transport through it.

Electrodeposition

On the more applied side, many posters were presented on various aspects of electrodeposition. In this field one can distinguish between the initial step and the growth process. When deposition is carried out at potentials less cathodic than the equilibrium value (underpotential), monolayers or fractions of monolayers are deposited. By careful control of the potential the desired fractional coverage can be achieved. Conversely, if deposition is initiated at potentials more cathodic than the equilibrium value, nucleation results. Subsequent deposition of smooth coatings can be achieved by lowering the overvoltage from that required for nucleation. Representative posters were presented by workers at the Netherlands' University of Utrecht (M. Sluyters-Rehbach et al.), who analyzed potentiostatic current-time transients occurring during nucleation, C. Cachet et al. (Université Pierre et Marie Curie, Paris), who studied such transients for zinc deposition from alkaline solution, F.M. Romeo et al. (University of La Plata, Argentina), who studied electrode resistance changes during the underdeposition of metals produced by changes in the electronic properties of the substrate, and Kolb and Twomey (Fritz Haber Institute), who observed anion adsorption during underpotential deposition of Cu on Au and Pt single-crystal surfaces.

The only lecture concerned with ambient temperature electrodeposition was presented by E.B. Budevski (Bulgarian Academy of Sciences, Sofia). He was primarily concerned with the deposition of unconventional alloys—e.g., the formation of very thin alternate layers of two metals by selective underpotential plating. Correspondingly, the deposition of alloy nuclei might give rise to alloys with novel properties.

Since it was recognized by Senderoff and Mellors in the 1960's that the refractory metals could only be successfully plated from molten salts, primarily fluorides, not much activity has occurred in this field, partly because handling of molten fluorides at the required temperature of 750°C on an industrial scale is difficult, and partly because the immersion at this temperature of steel, a prime candidate for electroplating, changes its mechanical properties in an undesirable way. Recently the pace of research in this field has picked up, motivated by the realization that salts other than fluorides might be acceptable media and that the required temperature might thereby be lowered. Progress in this field was reviewed by K.H. Stern (NRL, Washington), who presented some recent results of D. Inman at Imperial College, London, which show the importance of nucleation control on the morphology of the metal coating, and Stern's own work,

which shows that refractory compounds, such as carbides and silicides, can be deposited from molten fluorides by the simultaneous reduction of $(\text{CO}_3)^{2-}$ and $(\text{SiF}_6)^{2-}$, respectively, and the metal.

Batteries, Fuel Cells, Materials

The last day of the conference was devoted to simultaneous sessions on batteries, fuel cells, and materials—the latter frequently related to the former. In the plenary lecture A.G. MacDiarmid (University of Pennsylvania, Philadelphia) reviewed films of conducting organic polymers which exhibit electronic conductivity more usually found in metals. The first of these materials studied was polyacetylene, doped to provide p- and n-type conductivity, but more recently other polymers, such as polypyrrole, polyparaphenylene, and polythiophene have also been investigated. The field has progressed sufficiently so that application of these materials as cathodes in rechargeable batteries, as sensors, and in the biomedical field are now being considered.

Oxide-conducting solid electrolytes, particularly stabilized zirconia, have long been used in a variety of applications, such as O_2 sensors at high temperatures, and hydrogen-oxygen fuel cells. C.G. Vayenas (University of Patras, Greece) reviewed progress in this field, and presented new and novel application of these materials for synthesis. For example, NH_3 can be converted to NO , methanol oxidized to formaldehyde, and H_2S oxidized to SO_2 , while power is simultaneously produced.

The obligatory review of new materials for batteries and fuel cells was presented by A.J. Appleby (Texas A&M University, College Station). The major fuel cells now under active development include phosphoric acid,

alkaline, and high temperature (e.g., molten carbonate). In all these the progress which has been recorded consists primarily of the results of careful attention to factors which tend to lengthen cell life and improve efficiency. Progress has been steady, if unspectacular, and the lure of widespread use is always around the corner.

Conclusion

This meeting provided an excellent opportunity for electrochemists from all over the world to gather and exchange information. Since this is the first ISE meeting which I have attended, I have no way of comparing it with previous ones, but the format, with relatively few well-chosen in-depth reviews of major topics, is certainly helpful in organizing one's acquisition of knowledge of perhaps otherwise unfamiliar topics. More specialized topics were treated in poster sessions for which most authors were on hand for discussions. One indication of the success of the conference is that attendance at the keynote lectures did not fall off during the week.

Two books of abstracts were published which include both lectures and posters. Information about these can be obtained from Dr. Rainer Engels, the secretary of ISE: P.O. Box 40, 6800 AA Arnhem, the Netherlands.

Participants at this conference were evidently looking forward to next year's meeting, and the Japanese were already promoting the 40th ISE meeting to be held in Kyoto in 1989.

3/15/88

The 5th International Topical Meeting on Photoacoustic and Photothermal Phenomena

by Jane K. Rice. Dr. Rice is with the Optical Diagnostics Section of Chemical Dynamics and Diagnostics Branch, Chemistry Division, Naval Research Laboratory, Washington, DC.

The 5th International Topical Meeting on Photoacoustic and Photothermal Phenomena was held at Universität Heidelberg in Heidelberg, West Germany, from 27 through 30 July, 1987. It was supported by Deutsche Forschungsgemeinschaft (DFG), Land Baden-Württemberg, and Universität Heidelberg. The sponsors

were Deutsche Bunsengesellschaft für Physikalische Chemie (DBG), Deutsche Physikalische Gesellschaft (DPG), European Physical Society (EPS), and Gesellschaft Deutscher Chemiker (GDCh) in cooperation with the Optical Society of America. The conference committee chairman and cochairman were West

Germany's P. Hess, Universität Heidelberg, and J. Pelzl, Universität Bochum.

There were approximately 250 participants with 35 percent coming from West Germany. Comprising approximately 10 percent each were representatives from France, the UK, and the US. Other countries represented were Canada, Japan, China, Switzerland, USSR, the Netherlands, Italy, Israel, Ireland, Romania, Belgium, Yugoslavia, Spain, Portugal, Australia, India, Sweden, Czechoslovakia, Bulgaria, Brazil, Hungary, Saudi Arabia, Finland, Denmark, Scotland, and Poland. Thirty countries sent representatives, making the conference truly international.

The purpose of the conference was to examine new applications of the nonfluorescent detection methods of photoacoustic and photothermal detection and to compare new developments in experimental techniques. These detection methods are useful for a variety of systems – i.e., gas, liquid, or solid phase – and samples may have low or high light-scattering properties. Recent advances in time-resolved photoacoustic spectroscopy (PAS) have allowed the study of kinetics and relaxation. These nonfluorescent detection techniques have also proven effective for many applications in nondestructive evaluation in the health science field and in the semiconductor field. The sensitivity of these techniques has led to several types of trace analysis applications. In addition, interest has remained strong in the detection of physical properties of materials in the physics field where the photoacoustic phenomenon has its origin.

There were two plenary lectures held sequentially every morning and every afternoon. Two oral sessions were held after the lectures, which ran concurrently in the morning and afternoon for a total of 65 10-minute talks. After the oral presentations, poster presentations were available for review. There were 107 posters given. Ten general categories were used by the conference organizers. These were:

- Kinetics and relaxation
- Experimental techniques
- Biological and medical application
- Microelectronics and semiconductors
- Ultrasonics and material characterization
- Trace analysis and detection
- Surfaces and thin films
- Spectroscopy
- Mass and heat transport
- Nondestructive evaluation.

I will report on the following sessions: kinetics and relaxation, biological applications, trace analysis and detection, surfaces and thin films, and nondestructive evaluation. I apologize in advance for any slant toward the area of physical chemistry.

The full proceedings of the conference are presented in Volume 58 of the Springer-Verlag series in Optical Sciences. This volume, *Photoacoustic and Photothermal Phenomena*, is edited by P. Hess and J. Pelzl.

Kinetics and Relaxation

G.J. Diebold from Brown University, Providence, Rhode Island, gave one of the plenary lectures in this area. His paper was titled "Applications of the photoacoustic effect to studies of chemical kinetics and photochemical reactions." The use of photoacoustic detection for monitoring reaction rates affords the advantage that it is highly sensitive. Diebold reported that in a 1-photon absorption process this method gains a factor of 100 in sensitivity over using a Gilford Model 250 spectrophotometer. With lower concentrations of reactants, the rate of reaction is slowed and can be monitored easily. This allows one to bypass the problems associated with mixing reactants on a fast time scale. Several reactions were studied using PAS. These included inorganic species containing Co reacting with diphos and the photodissociation of dioxine. Two different applications were also addressed. The first involved the measurement of isotope effects using a chemically amplified photoacoustic signal and the second was a theoretical treatment for the photoacoustic effect produced by spherical particles.

A report on the reaction, $\text{BrNO} + \text{Br} \rightarrow \text{Br}_2 + \text{NO}$, was presented by K. Koseki, M. Koshi, and H. Matsui from the University of Tokyo. They determined a rate constant of $k_1 = 0.20 \mu\text{sec}^{-1} \text{ torr}^{-1}$ and an activation energy of $1.27 \pm 0.4 \text{ kcal}$. Koshi, Koseki, Matsui, and M. Yoshimura presented a study on the vibrational relaxation of silane and its fluorine substituents by time-resolved photoacoustic techniques.

A.C. Tam and H. Sontag from IBM-San Jose, California, and P. Hess from Universität Heidelberg presented a study of energy relaxation in CS_2 and NO_2O_4 vapors following 337-nm laser excitation. With pressures above 10 torr, photodissociation of CS_2 produces larger particles, yielding a slow heat-release component in the photothermal signal. Other collisional processes produce heat on a relatively faster time scale. This allows for a measurement of the rate of formation of the larger particles. In a separate experiment, transport properties (i.e., thermal diffusivity) of the $\text{NO}_2\text{-N}_2\text{O}_4$ vapors were measured as a function of pressure to study the effect of the chemical equilibrium on these properties.

Other reports included a time-resolved thermal lensing study of the photosensitization of singlet oxygen by R.W. Redmond and S.E. Braslavsky from the Max Planck Institute (MPI) at Mulheim, West Germany, and a study of complex specific heat in the glass transition regime by

B. Büchner and P. Korpium of Universität München, West Germany.

Biological Applications

S.E. Braslavsky from MPI at Mülheim began with a plenary lecture on the study of relaxation processes in biological systems and molecules of biological interest using time-resolved thermal lensing and photoacoustic spectroscopy. These detection techniques allow examination of large nonfluorescent chromophores, opaque samples, and *in vivo* measurements. The molecules studied by her group are large chromophores involved in photosynthesis – i.e., the light sensor, phytochrome, and the light transducer, chlorophyll-a. Much of the new work is based on new developments in time-resolved measurements. Between the time frame of heat delivery to the sample via laser absorption, which is on the order of 10 nanoseconds, and the thermal or acoustic dissipation in the liquid samples, which is on the order of milliseconds, the time frame for many chemical reaction or relaxation processes occur.

The second plenary lecture in this area was given by R.M. Leblanc from Université du Québec a Trois-Rivières, Canada, who discussed studies done on the chromophores involved in visual transduction and photosynthesis. In the visual pigment area, he has done low-temperature studies and also photoacoustic spectroscopy on intact retinas.

Trace Analysis and Detection

M.W. Sigrist of the Institute of Quantum Electronics in Zürich, Switzerland, gave a plenary lecture titled "Atmospheric Trace Gas Monitoring by Laser Photoacoustic Spectroscopy." In addition to sensitivity arguments, there are three advantages to using PAS for these studies. Firstly, the large dynamic range allows for low-concentration and high-concentration measurements of pollutants with the same equipment. Secondly, due to characteristic absorbances in the mid-IR range, one apparatus can measure many substances, and thirdly, *in situ* monitoring can be performed. Air pollution studies in a stationary CO laser unit and a mobile CO₂ laser unit are being performed. Ninety transitions have been observed in the range of 5.2 to 6.4 μm with the CO unit, which detects contaminants such as nitric oxides, aldehydes, propylene, and ammonia with a detection limit of 10 ppb. The CO₂ laser unit is mobile and is driven to various locations for continuous collection of data on airborne pollutants. A minimum detection concentration of 5 ppb has been obtained for ethylene in urban air. Other species detected are 1,3 butadiene, trichloroethylene, perchloroethylene, ozone, ammonia, toluene, and benzene.

Surfaces and Thin Films

Interesting medical applications were presented in the plenary lecture by P.E. Dyer from the University of Hull, UK, on excimer laser photoablation applied to cornea repair, laser surgery, and removing artery blockages in vascular tissue. The issues discussed were control of the rate and depth of ablation, and developing an understanding of the stress generated and the thermoelasticity of the tissue. Pressure generation of approximately 10^8 Pa with a fluence of 10-1000 mJ/cm^2 are being investigated. It has been found that the excimer laser creates faster ablation than the CO₂ laser, and therefore it is speculated that by use of this method chemical bonds are being broken. The CO₂ laser is absorbed by H₂O in the tissue and results in unwanted cell damage, whereas the ArF line of the excimer is not resonant with a H₂O absorption. It is hoped that some distinction can be made based on ablation threshold energies between healthy and diseased tissue.

Nondestructive Evaluation

A plenary lecture titled "Photothermal imaging with sub-100-Å spatial resolution," was given by a group from IBM-Yorktown Heights, New York. A micropipet outfitted with a thermocouple is used to sense a thermally, or optically heated sample with sub-100-Å spatial resolution. It is, in essence, a thermal microscope which can be used for temperature mapping. Additionally, when the sample is coated with gold, the investigator is able to obtain topographical as well as thermal resolution.

Another application on nondestructive evaluation techniques, presented by A.C. Tam and G. Ayers of IBM-San Jose, is to use ultrasonic imaging on layered structures to ascertain their thickness and perfection. Tam and Ayers can detect and identify multiple echoes from thin-layers that are several millimeters below the surface.

A theoretical plenary lecture on the mechanisms for the generation and scattering of sound and thermal waves in thermoacoustic microscopes was presented by L.D. Favro of Wayne State University, Detroit, Michigan.

Conclusion

This conference, the fifth in the annual series, had a large number of dedicated participants eager to discuss their many new technical advances and a number of new fields of application. Photoacoustic and photothermal detection methods have a stronghold in the measurement of atypical samples – i.e., *in vivo*, opaque, large non-fluorescent chromophores, and surfaces and subsurfaces which require a nonintrusive method of examination. The advances in the area of microscopy are impressive, and this area is growing. Although the conference covered a large number of technical advances and scientific applications and the participants spanned the fields

of physics, chemistry, medicine, and material sciences the conference still had a cohesiveness which was somewhat inexplicable and, as an indication of its strength, there was

a good deal of enthusiasm in planning next year's meeting.

3/22/88

COMPUTER SCIENCES

Engineering Applications of Transputers Initiative

by J.F. Blackburn. Dr. Blackburn is the London representative of the Commerce Department for industrial assessment in computer science and telecommunications.

Introduction

In February 1987 the Science and Engineering Research Council (SERC) and the Department of Trade and Industry (DTI) approved funding of £3.5 million (\$6.2 million) for a 4-year program on the development of engineering applications of transputers (see ESN 40-9:306-309 [1986] for previous article on transputers). The main objectives of the program are:

- To promote awareness of the potential of the transputer and associated technology
- To enable researchers to acquire the techniques, development tools, and systems software for using transputers in a quick and cost-effective manner
- To promote high-quality research using transputers without unnecessary duplication
- To transfer as early as possible the benefits of the research to UK industry.

The Rutherford Appleton Laboratory (RAL) Engineering Board's Distributed Computing Systems (DCS) program ran from 1977 to 1984. This led to a research community in the UK interested in the theory of parallel computing. An important theme of DCS was in loosely coupled distributed systems where many processors could be connected to tackle a specific problem in a flexible way. With large-scale integration, machines could be composed of many self-contained processors, each with its own memory, and could become more powerful, reliable, and cheaper than conventional computers.

In order to use such a machine effectively it must be possible to program it so that processors can share the work by communicating and synchronizing with each other. The system should be able to cope with the malfunctioning of individual processors. If each of the processors is identical it will be possible to reconfigure the system and provide a more fault-tolerant system.

Background: Transputers and Occam

In 1978, Professor Hoare of Oxford University proposed a model of computation called Communicating Sequential Processes (CSP), which concentrated on input, output, and concurrency as the basic primitives. Messages passed between processes were the basic method of communication, and these were synchronized so that the sender waits until the message is received.

Using these concepts, Inmos Ltd. developed a microcomputer, called the "transputer," designed for building high-performance computer systems. Inmos also designed a language, "Occam" (see ESN 40-9:306-309 [1986]), which implements Hoare's CSP theory. The transputer can carry out a set of concurrent processes with special instructions—sharing the processor time between the concurrent processes—and perform inter-process communication. Its external behavior corresponds to a process so that transputers can be linked with interprocess communication in a way similar to communication inside an individual transputer. Occam defines the computation to be performed as a collection of concurrent processes communicating with each other through channels. An Occam program can be executed by a single transputer, a small network of transputers, or a much larger network. Since a collection of processes is itself a process, an application can be defined hierarchically with a manageable set of processes being defined at each level.

RAL is providing support for an Alvey-funded research project, "The Transformation and Verification of Occam Programs," between Oxford University and Inmos Ltd. Since Occam is derived from Hoare's CSP, it is possible to define a set of laws between Occam programs which can be used as the basis of an automated transformation system. It is possible to define transformations of the original program which guarantee that the new

program has the same meaning as the original one. This can be used for improving the efficiency of the program, to show two programs are equivalent, and to transform to a restricted syntax for VLSI implementation. A prototype system has been written in the language Edinburgh Standard ML, which can transform Occam programs to a normal form.

Progress Report, First Six Months

A coordination team was established in the Information Division at the Rutherford Appleton Laboratory as soon as the first phase of funding for the program was approved. The main activities have been to publicize the initiative; to set up the Loan Pool and bring it into operation; to organize the tendering exercise for the national and regional centers and set up the centers at the selected sites; and to let development contracts for the production of key base software.

The Loan Pool, available only to the academic community, began operation in May, 1987. It now consists of Inmos and Meiko Company equipment only. To date, 48 loans have been approved from a total of 68 applications. The program allowed for access to the Loan Pool by users not normally supported by the Engineering Board, to a maximum level of 20 percent. Nine of the approved loans are in this category.

The tender for the National and Regional Support Center produced 23 bids. Invitations to tender were sent to all appropriate Academic Institutions. The chosen locations are as follows:

- Northeast Regional Center, Sheffield University, Director: Professor D. Lewin
- Northwest Regional Center, Liverpool University, Director: Professor W. Eccleston
- Scottish Regional Center, Strathclyde University, Director: Professor T. Durrani
- Southeast and Midlands Regional Center, Rutherford Appleton Laboratory (interim), Director: Dr. C.P. Wadsworth
- South, Southwest and South Wales Regional Center, Southampton University, Director: Professor A.J.G. Hay.

No decision has been made for the Southeast or Midlands, hence RAL is acting as the interim center. All the above listed centers began operation on 1 October 1987.

Five development contracts have already been let to begin to ensure that vital base software is produced to facilitate the exploitation of transputers in real engineering applications:

- Evaluation of Suitable Algorithms for Multi-transputer Arrays (Liverpool University)
- Define and Review an Occam Binding for the Graphical Kernel System (GKS) and Implement Minimal Level on GKS Using the Binding (University of East Anglia)

- Develop Finite Element Software for Multi-Transputer Arrays from Experience Gained on the DAP at Queen Mary College, London (Liverpool University)
- Feasibility Study into a Parallel Extracting Fortran Compiler for Transputer System Target (Brunel University)
- Software Migration Aids for Transputer Systems
 - a. Development of Standard Occam Harnesses for Processor Farm and Geometric Parallelism
 - b. Production of a User Guide to Occam and Transputers (Southampton University).

A 2-day workshop on transputer development environments was held 30 November and 1 December 1987 to survey the current situations, decide on what needs to be done to ensure that effective development environments are developed as quickly as possible, and to agree on who will accept responsibility for providing them.

Publicity has been an important component of the initiative and a regular mailshot has been established with currently 800 on the mailing list. SERC issued a press release in April 1987 formally announcing the approval of the first phase of the initiative. Also, members of the coordination team have given a number of invited talks at conferences and other meetings, and in all cases the initiative has been enthusiastically welcomed.

Occam User Group

The Occam User Group is an informal organization run by its own members. Its primary concern is the Occam programming language, developed by Inmos. But the hardware of the transputer is also an area of interest. The User Group acts as a forum for the interchange of information among existing and potential users of the transputer and Occam and as a channel for communication with Inmos. These aims are met by organizing meetings, issuing a newsletter, and supporting the exchange of programs between members. Technical meetings are held twice yearly, in March and September. They include informal presentations and demonstrations by members and by Inmos. There are special interest groups in Artificial Intelligence, learning, operating systems, formal aspects, networks, transputer hardware graphics, numerical methods and the Unix operating system.

The User Group maintains a catalogue, and through the newsletter, allows members to publicize programs that they are willing to make available.

Edinburgh Concurrent Supercomputer

A multimillion dollar installation, built by Meiko Ltd and based on transputers, is supported by DTI, the Computer Board, SERC and industry. (See article following for full description.) It is a large reconfigurable array of

Inmos floating-point transputers, with several hundred megawords of fast memory and a distributed file system, providing supercomputer performance. It is suitable for a wide range of applications.

Future Activities of the Engineering Applications Initiative

The most urgent requirement is to bring the regional centers up to their full operational level as quickly as possible. This is to ensure that the impact on UK industry will begin to take effect in 1988/89.

Associated support centers are to be introduced after 1 April 1988. At least eight such centers are to be established during 1988/89 with the Initiative contributing equipment but no manpower. The Daresbury Laboratory has already been established as an Associated Support Center to ensure maximum cooperation between the Initiative and the work at Daresbury on the Floating Point System T-20 machine. A limited configuration Meiko machine has been provided by the Initiative. Software developed for the T-20 will be ported to the Meiko machine and will be made generally available to the engineering community. Engineers can also have access to the T-20 systems as part of this arrangement.

The Loan Pool will be increased in both size and range of software and hardware offered. Many new developments have occurred since the start of the program – e.g., announcement of the T800 Floating Point Transputer. However, limited funds have restricted the range of equipment currently offered. The policy of providing only commercially available products will continue.

Further and extended development contracts will be let to ensure the usability of multitransputer systems in real applications. This will ensure use of these systems by UK industry.

Comments

It is unusual for the UK Government to support the launch of a product to the extent it is promoting the Inmos Transputer. In addition to the allocation of £3.5 million for the development of engineering applications a greater amount of funding through the Alvey Program has supported, in part, the Flagship Project at Imperial College London and the Supercomputer Project at the University of Southampton. Both of these projects are based on the Inmos transputer. Apart from UK Government support the transputer product is doing quite well. As of September 1987 there were 37 announced hardware products based on the transputer in the UK, US, Japan, and West Germany. Furthermore, there were 38 products and projects under development in the UK, US, France, and the EEC based on the transputer.

Prominent among the announced hardware products are those of the Meiko Company (see ESNIB 88-02:30-33). The Meiko M40 Computing Surface Module yields 1.1 billion instructions per second with 42 megabytes of concurrently accessed dynamic RAM. The effective bandwidth of the store is 24 gigabytes per second. A smaller desktop module, the M10, can deliver 250 MIPS and provides a compatible personal computer for workstation or development use.

2/15/88

The Edinburgh Concurrent Supercomputer Center

J.F. Blackburn

A multimillion dollar concurrent supercomputer which is based on transputers and built by the UK's Meiko company is being installed at the Edinburgh Concurrent Supercomputer Center, which is staffed by Edinburgh University personnel. The installation is supported by the Department of Trade and Industry (DTI), the Computer Board, the Science and Engineering Research Council (SERC) and industry. The computer is Meiko's model M40 Computing Surface Module, which is expected to yield 1.1 billion instructions per second. It has 42 megabytes of concurrently accessed dynamic RAM. The

effective bandwidth of the store is 24 gigabytes per second.

The first installment of DTI support, £575,000 (about \$1 billion), enabled the Edinburgh Center to procure a 32-processor system for programing development, each processor having 3 megabytes of memory. The system also has four display systems, 4.6 gigabytes of disk storage, communications and control for intercabinet communication, and eight disk control boards, each with 8 megabytes. This new hardware was integrated with the demonstration system – an M10 system – which had been installed 15 months earlier. The Computer Board sup-

port of £250,000 was used to purchase floating point T800 processors to replace the earlier T414 models. This upgrade was effected in October 1987.

The first release of software which permits division and allocation of the system's resources was installed in late 1987. The M40 uses a micro Vax as an attached support processor. Allocation of the fraction of the M40 specified by the user will be implemented as a part of the second release of the above-mentioned software.

Following is a review of the center's various programming developments.

Software

The first version of multiops, a multiuser version of the Occam programming system has been installed. With this version, up to 32 users will be able to edit, compile, and run code simultaneously. Each user is automatically allocated a separate transputer by the system when he logs on. In this first version of multiops, all files are held in the attached micro Vax, and are transferred to the M40 via an IEEE interface when required. When the file system software for the ECS's own half-gigabyte disks is complete, user files will be moved onto these disks. This will increase the bandwidth of the system.

The M40 is electronically reconfigurable. A software package which is being written will read a placement description from a file and map it onto the machine, setting the link switches as it does so, thus achieving a reconfiguration of the M40, as required by the user. Other software utilities that were available, as of late 1987, included a file transfer facility which enables users to move operational files from the microvax to a personal computer, and a screen dump facility which allows users to save images displayed on the high-resolution graphics monitors. As part of the software development effort at the University of Edinburgh, a standard set of graphics utilities has been developed for the Meiko MK015 graphics board. These drawing utilities do not include picture construction and manipulation facilities. However, they allow complicated two-dimensional images to be created and stored.

The graphics system is built in several layers. At the lowest level it is a collection of Occam 2 procedures which manipulate the MK015 graphics board directly. These procedures are able to:

- Draw lines, boxes, circles, arrows, and other simple geometric figures
- Copy portions of the screen
- Examine or change the color values stored in the color look-up table
- Display text in a variety of user-selectable fonts
- Store the current screen image in a file, or restore an image from a file.

The operation of the low-level graphics primitives is controlled by a set of parameters which users can modify.

Error reporting can be turned on or off, different fonts can be used, and clipping can be enabled or disabled. Most importantly, the system can draw pictures with either 8 bits of color resolution per pixel, or the full 24 bits. In 24-bit mode, each pixel can be assigned independent red, green, and blue values, so that 2^{24} different colors can be produced. In 8-bit mode only 256 colors are available at any given time, but the MK015's video memory can be divided into several frames. Each frame can be drawn on or displayed separately, so that users can create animated image sequences.

A set of interface procedures focus the second layer of the graphics system. These interfaces can be used by processes external to the MK015 graphics board to call the graphics system procedures. Each interface procedure handles the details of communication with one or more drawing procedures. A similar set of interface routings is provided to communicate with the graphics mouse handler. Finally, several template procedures illustrating the use of the graphics system are provided so that users can familiarize themselves with its use. This graphics system, called gfx, will eventually be incorporated into the standard Meiko software library. A user's guide to gfx has been prepared.

Occam 2 is usually written using the ops "folding" editor. When a group of lines is folded up it disappears from view, and is replaced by a single comment line. Folding is a useful way of representing complicated hierarchical structures, such as programs, as text. Folding allows the top-down design of programs to be visible once programs have been finished, since folds can be used to hide details of a particular implementation.

The only facility now available for printing Occam 2 programs destroys the fold structure. In addition, the existing list facility, called tds, can only display entire files, not selected portions of files. The University of Edinburgh is developing a new lister which preserves more of the program structure. Individual users can configure the lister so as to produce output in the form they find most readable. Output can also be formatted to be compatible with most common printing devices. The new lister is suitable for use in both the tds-2 and ops environments, and is near completion.

Applications Neural Networks

Neural networks are models of computation in which the single processor and large memory of a conventional computer are replaced by thousands or millions of simple interconnected nodes. Each node stores a single value and repeatedly updates that value according to the values of the nodes to which it is connected. Neural networks have achieved significant successes during the past few years in pattern recognition. A single transputer implementation of such a simulation has been developed in the Physics Department at Edinburgh, and is now being

transferred to the full M40 Computing Surface. This implementation learns to recognize and analyze pictures after having been exposed to sample pictures from a training set. The algorithm used in this simulation is called back propagation. In this algorithm the neural network's nodes are divided into several layers. Nodes in one layer are connected to nodes in the preceding and following layers by weighted links. These connections are represented as a matrix M , where M_{ij} is the strength of the connection between the i^{th} node of the first layer and the j^{th} node of the next.

Parallelism is introduced into this algorithm in two ways. First, the matrix multiplication which produces the states of the nodes in the $(j+1)^{\text{th}}$ layer from the weight matrix M and the states of the nodes in the j^{th} layer is done in parallel. Second, the network is exposed to all the pictures in the training set before it updates its weights. The various matrix multiplications can be done in parallel, and the results obtained summed on completion of the training set. This double decomposition is being used to divide the processing among the available transputers. The transputers are split into N groups, each of which deals with a subset of the training set of pictures. Within each group, the matrix multiplication is split up so that work is shared evenly among the transputers. This decomposition of the problem will allow the system to be tuned once the simulation has been transferred to the Computing Surface by increasing or decreasing the relative number of nodes in each group or subgroup.

Simulation for Quantum Chromodynamics

Quantum chromodynamics (QCD) is a physical theory which describes how particles interact in the nuclei of atoms. According to nuclear physics, the fundamental building blocks of matter are electrons and quarks. Electrons form the exterior of an atom, and are bound to the atom's nucleus by electrodynamic forces. These forces are described by quantum electrodynamics (QED).

The behavior of the protons, neutrons, and other nuclear particles made up of quarks is less well understood. While QCD predicts how quarks interact, the theory is not computationally tractable. It is believed that the intractability arises as a result of seeking to apply QCD at inappropriately small distance scales. There are reasons to believe that no current theory is valid at the smallest length scales. Lattice quantum chromodynamics seeks to limit the scope of the theory by approximating the space-time continuum as a discrete four-dimensional lattice of points, thus excluding all phenomena below the scale of the lattice grid spacing. This restores computational tractability, and should allow predictions for physical quantities such as the proton mass to be extracted from the theory. Comparison of these predictions with experimental values will allow the theory to be verified or

refuted. Simulations on even very small lattices still require enormous amounts of memory and computation. On each link of a QCD lattice there is an 18-element matrix representing a particular field variable. Using 32-bit arithmetic, even a very coarse grid containing only four points in each of the four space-time directions requires 72 kilobytes to store the value of just this one variable. The aim of the work with the Computing Surface is to develop simulations on a $32 \times 32 \times 32 \times 32$ grid, which will require almost 300 megabytes of memory. The program being written allows a large lattice such as this to be spread across a network of transputers in various ways. There is expectation that results from large lattices may provide the first significant tests of the accuracy and validity of the current theories of matter.

Medical Imaging

A medical imaging system to aid radiologists in interpreting three-dimensional nuclear magnetic resonance (NMR) images is being developed using the M40 Computing Surface. The bulk of the programming effort is being carried out by postgraduate students from Computing Science and Artificial Intelligence as part of their theses, and a full demonstration system is in operation. When using NMR images directly, even a trained radiologist has difficulty picturing a three-dimensional object based on several slices through it. Another difficulty is the sheer amount of data NMR provides. While two or three slices viewed in conjunction can improve a radiologist's knowledge of the object, a dozen or more slices become confusing. The program being developed allows the user to examine the NMR image data as two-dimensional slices, or to examine selected portions of it using a three-dimensional display capability. Once part of a surface or volume of interest has been selected by the user, the rest of that surface or volume is found by the program, and displayed on a high-resolution color monitor. Several surfaces or objects can be displayed simultaneously, and various combining operations performed on them. The parallelism of the Computing Surface is exploited in several ways by this program. At the image processing level, the NMR data is distributed among the available processors. All of these processors then track the surface or volume of interest simultaneously. With N processors, this results in a processing speedup of almost N times.

Parallelism is exploited again in the display portion of the program. The object found is represented as a set of polygons. These polygons must be transformed from three dimensions into two dimensions, shaded, and displayed on the graphics monitor. Much of the calculation involved in this can be done independently for each polygon, therefore a load-balancing network of transputers is used.

The plan is to make this program a marketable medical imaging system.

Fluid Flow Simulation – Cellular Automata

The behavior of fluids is described by a set of differential equations, known as Navier-Stokes equations. These equations can be solved exactly when the fluid flow is smooth. However, it becomes difficult to solve them when they describe fluids which are flowing past barriers, or fluids in which vortices or shock waves exist. Therefore, most practical analysis of fluid behavior must be done using simulation. The technique in the past has been to approximate the solution of the Navier-Stokes equations. However, for complex systems the amount of calculation required is prohibitive. A new technique based on mathematical objects known as cellular automata, is now being investigated as a way to simulate larger and more complex fluid systems.

In its simplest form, a cellular automata is a line of sites. Each site can store a single value, known as its state. At regular time intervals the values of the sites are simultaneously updated according to a rule whose result depends on the previous state of the site and on the status of the neighboring sites. If the state of site C_i at any time (t) is either 0 or 1, the state of that site at time $t + 1$ could be given by

$$C_i(t+1) = (C_{i-1}(t) + C_{i+1}(t)) \text{rem} 2,$$

where rem is the remainder function. A cellular automata using this rule evolves as shown in Figure 1, where each successive row is an image of the cellular automata at a successive time step. White represents sites with value 1, while black represents sites with value 0. These ideas can be extended to create multidimensional cellular automata. A two-dimensional cellular automata is made up of many identical sites placed at the vertices

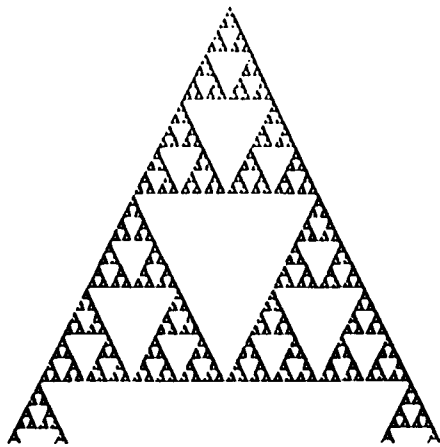


Figure 1. Evolution of 1-Dimensional CA.

of a regular planar grid. At each time step, each site updates its state according to the states of some or all of its neighbors. The update rule is the same for each site in the system, only the values of the sites differ. Cellular automata in three or more dimensions can be created by using higher dimensional grids. The most famous cellular automata is Conway's "Game of Life," which uses a square two-dimensional grid of sites, each of which is either alive or dead. The update rule counts the number of live sites adjacent to a particular site C_{ij} , and makes C_{ij} alive on the next time step if the number of live neighbors is between certain thresholds. Complicated and unpredictable patterns can be produced using this very simple rule. Cellular automata are an efficient method of modeling the Navier-Stokes equations. Each site of the cellular automata simulates a location in space which may be occupied by zero or more particles moving along the links connecting the sites. The number of particles occupying a site at a given time, and their direction, determines the state of the site at that time. An exclusion rule is enforced to prevent two particles moving in the same direction from occupying the same site at the same time, since such particles would be indistinguishable.

The state of a site can be encoded as a binary number, with one bit of the number used to represent each of the links connecting the site to its neighbors. If the bit is a 1, then there is a particle moving out on that link. If the bit is a 0, the link is empty. Sites can then be updated by comparing their states with the states of their neighbors; no explicit modeling of particle motion needs to be done.

A cellular automata of the type described is an example of a lattice gas model of liquid dynamics. Lattice gases model an idealized world in which all particles are the same size, and move with the same speed. The only things which distinguish particles are their locations and the directions in which they are moving. It has been shown by averaging particle density and momentum over large enough areas of the cellular automata, the behavior described by the Navier-Stokes equations can be recovered. This means that cellular automata of the correct type, while highly idealized, are nevertheless good enough simulations to reproduce the behavior of interest.

The Hardy Pazzis Pomeau (HPP) Lattice Gas Model

The first hydrodynamic cellular automata model started out as a mathematical investigation of the properties of a lattice gas by the Center's J. Hardy, O. de Pazzis, and Y. Pomeau. The HPP Model used a square two-dimensional grid on which identical particles moved with a velocity of one link per time step. Up to four particles could reside at each vertex at any instant. An exclusion rule was enforced which prohibited the simultaneous occupation of a site by indistinguishable particles – i.e., par-

cles occupying the same location and moving in the same direction. In updating, particles were moved one step from their current site along the appropriate link to a neighboring site (this means that the values of sites were updated to reflect interactions between those sites and their neighbors). Collisions between particles now occupying the same site were then resolved to determine the directions in which those particles would move at the next instant. In general, of the many possible rules for updating the configuration of a site at which a collision is occurring, only a few rules lead to physically correct, and computationally efficient systems. For example, two particles colliding head-on could be replaced by a single stationary particle, by two particles moving off in directions opposite to the direction of the original particles or moving at right angles to the first pair. The first rule does not conserve the total number of particles in the system, and so is physically incorrect. The second rule, while physically correct, does not produce interesting overall behavior, because the result of the collision is indistinguishable from what would have happened if the particles had missed each other and not collided at all. Only the third rule is useful to implement. This model was able to satisfactorily simulate sound wave propagation, but the underlying square lattice contained insufficient symmetries to yield the correct form of the Navier-Stokes equations. Obstacles tended to cast shadow, rather than produce vertices.

The Frisch Hasslacher Pomeau (FHP) Method

The FHP, a more refined model, proposed in 1986, uses a regular hexagonal lattice, which allows for a more complex set of collision rules. The HPP method is deterministic in that for every pre-update site configuration there is exactly one post-update site configuration. But with the hexagonal lattice, it is possible to have more than one valid post-update configuration for some pre-update configurations. If the selection of one of these post-update configurations is made randomly each time a collision occurs, the model is nondeterministic, i.e., nonrepeatable. Alternatively the model can be made deterministic by always choosing the same post-update configuration for any pre-update configuration. The generalization of these two-dimensional models to three dimensions is not trivial because no regular lattice in three dimensions has the required amount of symmetry. One possible approach is to use a multispeed model on the regular cubic lattice, allowing rest particles, particles moving with unit velocity along the links of the cubic lattice, and particles moving diagonally with velocities of $\sqrt{2}$. Another promising approach is to use a four-dimensional lattice, and then project it into three dimensions. These models and others are under investigation.

Implementing a Lattice Gas

The natural way to distribute the task of processing a large lattice system with only local interactions, like the cellular automata fluid model, is geometrical decomposition. Each transputer is allocated a physically contiguous segment of the lattice, which it is responsible for updating. The necessity for communicating the particles crossing the edges with a neighboring segment constrains neighboring transputers. This is achieved by having a chain of transputers, each of which is responsible for a long, narrow strip of the lattice. The workers in the chain are connected by a bidirectional data highway. The chain is controlled by a master processor located at its head. Data is passed toward the end of the chain along one set of channels, and towards the master processor on another set.

Two processes run concurrently on each worker transputer in the chain. The evolver process updates the sites in its own segment and processes them to produce the averaged velocities. This velocity data is then passed to a data passer process running on the same transputer, which merges the new data with that already on the data highway.

A single graphics processor connected directly to the system master interprets the data from the worker transputers and displays it on a high-resolution color monitor. This display process produces an animated frame-by-frame picture showing the current state of the fluid system.

Since the values of the sites on the edge of one transputer's region of the system must be communicated to that transputer's neighbors, there is a need for periodic synchronization. While this synchronization is efficient when the workloads of the transputers are balanced, it would be very inefficient with unbalanced workloads. In general, it is very inefficient to have the bulk of the transputers waiting for a few to finish processing excessive work loads, and far preferable to have a few processors sitting idle while the majority are busy computing. However, farming out jobs to achieve better load balancing would be disastrous in this application, since the amount of data to be transmitted would be very large, while the computations themselves are very simple.

The Computing Surface Implementation

In the system at Edinburgh, each of the 39 worker transputers is given a segment of the system, consisting of a vertical strip 30 cells high and a single cell wide. Each of these cells contains 12×12 cellular automata sites. Most of the simulation tests have been carried out using 39×30 cells — i.e., a 468×360 system of 170,000 sites. A few tests were done to determine the viability of the memory-bound maximum possible simulation of 60×60

sites per cell. These simulations were too slow to be useful (23 seconds per HPP evolution). This scale of simulation on 4.2 million sites is comparable with the simulations currently reported as standard by other research groups. While the square HPP lattice is naturally stored as a two-dimensional array, a subtle modification is required to store the FHP model's hexagonal lattice. This is achieved by introducing diagonal connections between certain sites, but not between others, so as to give each site six neighbors.

The Edinburgh simulation also permits free specification of the state of the system, at the start or during a run, allowing barriers or particle sources to be specified on sites within regions selected using the mouse. As well as determining the type of wake expected behind arbitrary barrier systems, the type of flow can thus be modified, greatly enhancing the modeling possibilities of the simulation.

Collision rule update is handled by table look-ups, and the fully nondeterministic version is in operation. Movement shifts the particle from a specified site configuration to the appropriate configuration on the neighboring sites. The update of all of the sites in the system is done by sweeping through all of the sites sequentially on a particular transputer, but evolving each transputer concurrently. The states of the sites on the edges of the segments are required by their neighboring segments. This is handled by allowing particles to move all the local lattices into special "holds," which are then communicated and merged with the sites on the edge of their neighbors. A natural synchronization of neighboring transputers takes place when this edge information is exchanged after each update, but the averaged information sent on to the data highway is completely independent and run in parallel with the evolver. The system used has default-reflecting boundaries on all of its edges. The reflecting boundary is a line of special wall sites on each edge which blocks the path of particles attempting to move onto them. A particle can either be sent back along the direction from which it came or specularly reflected about a normal to the barrier. Alternatively, some proportion of both of these rules could be used, resulting in a diffusive boundary. Although a smooth, perfectly reflecting boundary may seem the most natural, this boundary is, in

fact, generally nonphysical, in that at the molecular level all surfaces are basically rough, and slow down particles in the wall region. Special sites are also required which add particles to the system and remove particles from it. By placing these appropriately, flows of particular interest can be created.

Results

The current average transputer evolution speed is 74 microseconds/site. However, since 39 transputers are processing simultaneously in the Edinburgh Center's supercomputer, the equivalent sequential performance of the Computing Surface is 1.9 microseconds/site.

Several simulations were made using the HPP model, but only the shock-type simulations could be considered realistic, particularly the central spherical shell shocks. The FHP Model as implemented has been used for a wide range of simulations including:

- A range of shock simulations, including shock in a box
- Steady flow in a horizontal channel producing Poiseuille flow with the Slichting Velocity profile
- Choked channel flow within a steadily more confining channel for determining flow characteristics
- Von Karman vortex streets formed by flows obstructed by orthogonal barriers and oblique barriers
- Flow around sequences of barriers
- Crossflow into a channel in which a pipe introduces a jet orthogonal to the flow occupying a channel, forming vortices downstream.

The work has shown that cellular automata have the potential for accurately modeling a wide range of hydrodynamic phenomena. This simulation allows a large degree of freedom in the specification of a flow by its boundary conditions at no extra computational cost. This makes the system an interesting vehicle for implementing a numerical wind tunnel in which the behavior of fluids flowing around airfoils and other objects of interest can be economically studied.

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Edinburgh Concurrent Supercomputer Newsletter, Number 2, August, 1987, Edinburgh University Computing Service, Mayfield Road, Edinburgh, EH9 3JZ.

2/12/88

Vector and Parallel Processors in Computational Science III

J..F. Blackburn

Introduction

The third conference in the computational science series, held at 3-year intervals, took place in August 1987

at Liverpool, UK. It was attended by about 240 delegates, most of them from the UK, but there were some delegates and speakers from the US and some delegates from West

Germany. A selection of 14 papers from a total of 40 are summarized in the following paragraphs.

An Overview of Parallel Architectures

Professor P.C. Treleaven, University College London, UK, first addressed the Fifth Generation Computer development. He said that one aim of the development is to achieve intelligent consumer electronic products – e.g., a television system including interrogation. For this purpose artificial intelligence (AI) software is needed. The principal candidates are LISP and Prolog and their derivatives, but to efficiently run these languages new computer architecture is needed in computer hardware systems. Such architecture has resulted in parallel processor systems based on microelectronic building blocks – the transputer, for example. Various architectural choices have been made including those in LISP, reduction, and dataflow systems. The Japanese have chosen logic machine design to run Prolog or Prolog-derivative languages. The US was heavily committed to LISP before Prolog came along, and LISP is used in expert systems and connection machines. In Europe the emphasis is on reduction machines and functional languages. Treleaven then addressed other parallel computer areas. He said that:

1. Parallel transaction processing systems are exemplified by parallel Unix systems and communication systems like BBN's Butterfly.
2. Examples of numerical supercomputers are vector systems like Cray 2, array processors, and multiple-instruction multiple-data (MIMD) systems.
3. Very large scale integration (VLSI) systems include array and systolic systems, and microcomputers (e.g., transputers) connected in parallel.
4. High-level language machines include functional programming systems like ALICE and GRIP in the UK, and logic computers like the parallel inference machine in Japan and the multischuss of Bull Co. in France. Other examples include knowledge-based systems in the US and object-oriented systems like DOOM at Philips in the Netherlands, AOOM in Japan, and SOAR at the University of California, Berkeley.
5. New approaches include neural systems to act like the human brain as well as computers using new technologies like gallium arsenide chips, optical computers based on photons, and molecular computers.

In the near term, parallel computers will be fully commercialized and incrementally expandable. Over a 7- to 10-year period, systems with 1,000 to 10,000 microcomputers will be available, and there will be an increased interest in connection machines for special purposes. Finally, Treleaven said that within 15 years there will likely be available general purpose optical computers,

molecular processors, and connection machines based on neural networks.

Comparing Shared and Distributed Memory Machines

In his presentations, C. Baillie, California Institute of Technology, Pasadena, said that there are two distinct types of MIMD computers: the shared memory machine, (e.g., Butterfly, RPB) and the distributed memory machine (e.g., the hypercube, transputer array). Typically these machines use different programming models. The shared memory machine has monitors whereas the distributed memory machine uses message passing. Baillie spoke of the implementation of monitors on the Butterfly and message passing on the hypercube in some detail. This was followed by discussion on the advantages and disadvantages of these two methods of memory arrangement. One may think that a shared memory machine with monitors is simpler to program than a distributed memory machine (along with its host) using message passing, but this is not necessarily the case. A distributed memory machine can use message passing more efficiently than monitors but will a shared memory be more efficient with monitors or using message passing? The results of various benchmarks run on the Butterfly and hypercube were presented as evidence.

The Design Philosophy of DAP Prolog

The majority of work done on the implementation of Prolog, or a parallel dialect of Prolog, has emphasized the list-oriented nature of Prolog and neglects its database aspects, according to A. Bale and P. Kacsuk, Queen Mary College, London, UK. This is true despite the wide recognition of Prolog as an outstanding candidate for the realization of logical databases. The other main feature of present research in this field is its frequent reliance on modification of control mechanisms while not considering the modification of data structures.

The object of the project of the DAP Support Group at Queens College is the implementation of Prolog on a single-instruction, multiple-data (SIMD) type of computer called the Distributed Array Processor (DAP).

In a SIMD machine the main source of parallelism is the substitution of recursive or iterative loops by operations on regular data structures such as matrices. Therefore, to implement Prolog efficiently on the DAP we make use of the available parallelism by introducing some regular data structures into Prolog. To do this the data structures of conventional Prolog are extended with regular data structures such as sets and matrices, while the control mechanism is modified in different parts of a Prolog program to handle these new structures.

OCCAM and Other Parallel Languages

D. May, INMOS, Bristol, UK, said that OCCAM is based on the concepts of concurrency and communication. (See ESN 40-9:306-308 [1986] for previous discussion of OCCAM.) These are important concepts for systems built from multiple, interconnected transputers. The language is oriented toward interactive use, and it enables complex systems to be described in a concise and readable form. A process performs a sequence of actions and terminates. Each action may be an assignment, an input, or an output. An assignment changes the value of a variable, an input receives a value from the channel and an output sends a value to a channel. At any time between its start and termination a process may be ready and waiting to communicate on one or more of its channels. Communication is synchronous. When both an input process and an output process are ready to communicate on the same channel, the value to be output is copied from the output process to the input process. The input and output processes then continue.

Each channel provides a one-way connection between two concurrent processes, one of which may output to the channel and the other may input from it. When a process is waiting to input from more than one channel the input is taken from the first channel which is used for output by another process. OCCAM may be used to program a network of computers. Each computer with local store executes a process with local variables and each connection between two computers implements a channel between two processes.

Uniformly addressable memory space leads to problems in parallelism. To solve this problem each processor is provided with local memory. Arbitrarily large systems are allowed with localized communication. OCCAM can be considered as a high-level assembly language for parallel processing. Simulated and real concurrency ensure that the distributed system works efficiently. A language needs to be susceptible to mathematical testing for correctness.

In a parallel construct there is no sharing of variables, and communication is synchronized through communication channels. Concurrent processes can be interleaved in any order. Synchronized communication provides ease of implementation and efficiency through nonbuffered communication.

An Array Processing Language for Transputer Networks

At present, transputer networks are programed in OCCAM. The synchronous parallelism typical of array processing applications has to be programed using arrays of asynchronous OCCAM processes, distributed across the network. Data alignment operations, such as access-

ing a neighbor's data, must be coded as explicit input/output operations. With so much visible concurrency and communication, it is difficult to keep intellectual control of significant programs. After this review, D. Crooks, The Queens University of Belfast, UK, said that at Queens a higher level language called LATIN (language for transputer networks) has been developed. LATIN draws together two language approaches for expressing parallelism: (1) asynchronous MIMD processes as in CSP or OCCAM and (2) synchronous array processing-type SIMD parallelism, as in the Pascal-based array and vector processing language Actus. Thus, LATIN has both SIMD and MIMD parallelism. A single LATIN process can have an array processing capability, which is implemented automatically by an array of transputers. All the mapping of the data and code over this array is done by the compiler. As a result, for array processing applications, programing is faster and more reliable.

LATIN is being implemented by constructing a translator, which translates LATIN programs into OCCAM. Because OCCAM is close to the transputer machine code, this approach should not be less efficient than direct compilation, and will enable much more rapid implementation.

Fault-Tolerant, Self-Repairing Transputer Arrays

In addition to the use of transputer arrays to achieve higher speed in processing, another advantage is that of higher integrity. C.J. Elliott, Smith Associates, Cobham, UK, described a project for the European Space Agency to develop an onboard computer for satellite data processing. Three required constraints for computers on satellites are: space-qualified fabrication, radiation resistant, and fault tolerance. Transputers are used in this project with serial links and drivers, low chip count, and the OCCAM language.

An Architecture for a Multivector Processor System (VPP)

Recently many kinds of supercomputers based on vector and parallel processing have been proposed. Atsushi Inoue, Toshiba Corporation, Japan, described a flexible multivector processor system under development called VPP to be used for satellite image processing. The architecture of the system consists of many processing units (PU's), a high-speed connection network, and a front-end processor.

The PU is a vector processor which executes programs in the local memory on a MIMD basis. The PU can handle array indices explicitly. It can generate a set of indices which satisfy given conditions and execute vector operations with these sets of indices.

The high-speed network can connect up to 64 PU's and all PU's can send data simultaneously without any transfer contention. The network is designed to be implemented by gallium arsenide (GaAs) devices to achieve very high transfer capacity.

On the VPP system a program is divided into subprograms to each of which several PU's are assigned. The number assigned to a subprogram depends on the processing complexities of the subprogram. Data are sent successively to PU's where they are processed by the subprograms. Data appear to flow through a pipeline formed by the PU's. This so-called processor pipeline can be set suitably for different problems. From this it gets the name Variable Processor Pipeline (VPP).

The Megacell Machine

Hungary's megacell machine, according to T. Legendi, Hungarian Academy of Sciences, is a general-purpose highly parallel computing unit, called cellprocessor. It contains millions of parallel-working, identical Boolean processing elements, called microcells, and is modularly extendable. As a back-end processor of a traditional computing system, it can solve parallel-nature problems at a high speed and independently of the host computer.

Legendi described the architecture of the machine and discussed the possibility of LSI, VLSI, and WSI implementation. He also described the programing methodology and languages. Megacell applications include image processing, matrix operations, and finite element analysis.

A Benchmark of the SCS-40: A Minisupercomputer Compatible With the CRAY X-MP/24

An accurate benchmark of the SCS-40 minisupercomputer was described by H.J. Wasserman, Los Alamos National Laboratory, New Mexico. He said that the architecture is similar to that of supercomputers in that it has various levels of processor and memory parallelism. In particular, it is a vector processor. Through use of off-the-shelf electronic technology the minisupercomputers cost considerably less than true supercomputers. The SCS-40 uses an instruction set that is essentially a duplicate of that used on the CRAY X-MP/24. The benchmark results on the SCS-40 were compared with those of the Cray X-MP/24, the Alliant FX series, and the Convex C-1. The Alliant computer, a multiprocessor system, provides the only commercially available Fortran compiler that automatically partitions code for concurrent execution.

Evaluating Parallel Processors for Real-Time Applications

Increasing acceptance of the necessity for high-order parallelism in order to allow progress in digital processing still leaves open the large question of what machine architectures are best for which class of problem. J. Roberts of the UK's Royal Signals and Radar Establishment (RSRE) said that the RSRE is investigating and comparing the use of both SIMD and MIMD architectures for programmable processing in real-time systems. A distributed array machine, mil-DAP, derived from the ICL DAP, has been developed and benchmarked on radar, image processing, speech recognition, signal processing, and terrain modeling problems. Multi-transputer arrays have been applied to an overlapping set of problems in image processing, Fast Fourier Transform, and terrain-based computation. The results were compared and some preliminary conclusions were drawn.

The ESPRIT Transputer Project

C. Jesshope, Southampton University, UK, reviewed this project, saying that its objective is to develop a high-performance multiprocessor computer with supporting software and a range of applications to demonstrate its performance.

The project has had ESPRIT support for the past 18 months and has also had support from the UK Alvey Program in developing the first transputer supernode. Work under ESPRIT support began in December 1985. (See ESN's 37-12:447-450 [1983]; 39-1:12-13 [1985]; 39-6:252-55 [1985]; 40-11:411-14 [1986]; 40-11:414-19 [1986]; R-11-84; R-13-84; C-8-85 for reports on ESPRIT, Alvey, and T800.)

The latest models of the supernode use the INMOS T800 transputer (ESN 40-9:306-308 [1986]), which became available in January 1987. Three supernode models were demonstrated during the ESPRIT technical week in Brussels at the end of September.

The basic design of the system at Southampton is a modular, hierarchical architecture based on reconfigurable nodes of transputers. VLSI switches (designed at Southampton University) under transputer control determine the topology of the network within and between nodes. Reconfiguration can be done during program execution under the control of the programs.

A supernode consists of 16 worker transputers, each of which is a T800 which includes a 32-bit CPU, a 64-bit floating point unit, four standard transputer communication links, 4 kbytes of random access memory, a memory interface, and a peripheral interface on a single chip using a 1.5-micron CMOS process. The four links of each worker transputer are connected to a 72×72 VLSI switch

which is controlled by a further transputer with its links connected to the switch. The 72×72 switch is implemented in two Nippon Electric Company integrated circuits, each functionally equivalent to a 72×36 crossbar switch. Each T800 has 256 kbytes of external memory, and the node has an additional transputer with 16 mbytes of memory for storing and distributing data and code. A Winchester disk controlled by an M212 transputer can be included in the node. An internode switch is used to implement a three-stage network for reconfiguration between nodes.

A control bus enables any transputer to communicate with the control transputer independently of the links. This is used for synchronization and for debugging programs.

The reconfigurable transputer processor supports static, quasi-static, and dynamic operation of the switched system.

The T800 is capable of sustained floating point performance in excess of one megaflop per second, and the estimated performance of a supernode with 16 worker transputers is in excess of 16 megaflops per second.

Finally, Jesshope said that software is being developed for application in science and engineering, signal and image processing image syntheses, computer aided design, and computer aided manufacturing.

A Two-level Parallel Scheme for Two-Dimensional Hydrodynamics

The WAVE Code is a large, complex two-dimensional relativistic electromagnetic particle simulation code developed at Los Alamos National Laboratory. In his presentation, R.G. Babb said that the Laboratory's WAVE is used to study various linear and nonlinear plasma phenomena by solving Maxwell's equations and particle equations of motion on a Cartesian Mesh with a variety of fields and particle boundary conditions.

The code cannot easily be vectorized-one computational kernel had been previously hand coded in Cray Assembly Language (CAL). The objective of the work Babb described is to compare various approaches to speeding up the execution of this code using the following strategies:

- Compiler directives and minor code restructuring to increase vectorization
- Speedup through unassisted hand-coded CAL
- Speedup through use of SARA, a CAL coding tool that translates a single assignment CAL-like language into highly optimized CAL.

Results also compare the above versions for the Cray X-MP and SCS-10.

Computation With Symmetric, Positive-Definite, and Band Matrices

Computations involving symmetric, positive-definite, and band Matrices are kernel operations in the numerical treatment of many models arising in science and engineering. Z. Zlatev, Danish Computing Center, University of Copenhagen, began his talk by pointing out that a high level of performance is desirable when such operations are to be carried out on a vector processor. If the operations are performed by rows, then the loops are vectorized but the speed of computations, measured in megaflops, is not very high because the arrays involved are normally short. Therefore the computations should be carried out by diagonals. Also, some special devices are to be applied in order to enroll the loops. Finally, he said, the storage scheme requires care and planning. He demonstrated that if: (1) the computations are performed by diagonals, (2) the storage scheme is well chosen, and (3) the main loops are included then the speed of computation is nearly the same as that obtained in computations with dense matrices. The fact that the computations are performed by diagonals can be exploited to avoid computations with zero diagonals. Zlatev described kernel subroutines performing matrix-vector multiplications and gave numerical illustrations. The incorporation of these subroutines in solvers of linear algebraic equations based on a conjugate gradient algorithm was discussed. The effect of different preconditioners in the efforts to accelerate the speed of convergence was demonstrated by numerical experiments.

An Approach to Massive Parallel Multiprocessor Programming

Multiprocessor Systems, especially massively parallel multiprocessors, introduce new requirements that have not been encountered before. M. Adelantado, University of Toulouse, France, said that each problem must be partitioned into tasks and each task must be scheduled for execution, and also that synchronization of control and dataflow must be performed during execution. In order to achieve high performance, efficient solutions must be found to these requirements. The solution appears to be in the software development environment. A programming approach was described for solving large-scale numerical applications in a MIMD massively parallel area. The proposed programming tools satisfy the following requirements to:

- Develop a high-level and an attractive environment adapted to nondedicated machines
- Offer explicit tools which allow an efficient partitioning and parallelization of numerical problems
- Facilitate program development and debugging.

Adelantado suggested two-level programing methodology in which a high-level central language at the first level would allow expression of parallelism and, concurrency between tasks and at the second level, automatic tools would be used to detect fine-grained parallelism.

Comments

The papers presented at this conference covered parallel computer architecture, programing for parallel

systems, and the adaptability of a variety of applications to parallel processing. Their quality was generally high and the presentations were mainly quite effective.

This conference followed two successful conferences – VAPP I, in 1981 at Chester and VAPP II, in 1984 at Oxford. The proceedings of VAPP III will be published by North-Holland as a special issue of *Parallel Computing*, edited by L.M. Delves and R. Wait.

2/4/88

CONTROL SYSTEMS

High Quality Control Research at the Institute for Flight Systems Dynamics

by Daniel J. Collins. Dr. Collins is the Liaison Scientist for Aeronautics in Europe and the Middle East for the Office of Naval Research's London Branch Office. He is on leave until June 1988 from the Naval Postgraduate School where he is a Professor of Aeronautical Engineering.

The Institute for Flight Systems Dynamics (IDF), located in Oberepfaffenhofen, near Munich, is one of the 21 laboratories that make up the German Aerospace Research Establishment (DFVLR), which is the largest research establishment in West Germany.

Dr. J. Ackermann, director of IDF, told me that IDF's primary effort is in guidance and control of robots, surface vehicles, and dynamic systems (with particular reference to aerospace vehicles, robots, and ground vehicles). IDF is well equipped with the primary tools for this work – computer facilities which include a hybrid computer for real-time simulation of guidance and control systems, a process computer for investigating computer controlled systems, a robot laboratory, and graphic display stations for demonstrating three-dimensional motion. The institute, which has 74 employees of whom 47 are scientists, is organized into four groups; these groups (and their heads) are:

- Multibody dynamics (Dr. Wili Kortuem)
- Guidance (Dr. Klaus Well)
- Control (Professor Geog Gruebel)
- Automation (Dr. Gerd Hirzinger).

I shall report on the activities of each of the groups and list some of their current publications.

Multibody Dynamics

Dr. Kortuem, head of this group of 14, is presently at Stanford University in California. I talked to Mr. A. Jaschinski, who indicated that the group has been involved in simulation of complex systems such as magnetic lifting trains for over 10 years. One result of this activity is a set

of fairly extensive computer programs – FADYNA, MEDYNA, and MULTIBODY – which demonstrate the feasibility of the multibody approach. The code FADYNA is concerned with small deviations from a reference motion which simulate the dynamic motion of vehicles with flexible tracks. Its principle area of application has been with magnetically levitated vehicles with elevated flexible guideways. The successor to FADYNA is the computer code MEDYNA, which has a wide spectrum of modeling capabilities, efficient computational routines, and excellent graphics (Kortuem and Schiehl, 1985). It is especially suited for tracked surface vehicle systems. The MEDYNA code is now available commercially through DFVLR and New Technologies (MAN), a Munich company. Present input and outputs are in German or French, but there will be an English version before the end of the year. Preprocessors and interfaces for MEDYNA are being developed or are available for NASTRAN and for ACSL. Although forces can be nonlinear in MEDYNA, the code is essentially linear in the body displacements (small displacements). Work is now in progress to extend the code to nonlinear displacements which would have application to robotics. The third computer code, MULTIBODY, is concerned with large rotations of rigid multibody systems such as in satellite attitude dynamics.

Guidance

Dr. Well stated that the research activities of the guidance group were directed at the development and application of optimization methods for better system per-

formance and guidance of aircraft and missile systems. As in the case of the multibody dynamics group, general software – in this case for simulation and optimization of complex problems – is being developed. A differential equation solver called RKF45T has been developed to solve differential problems involving piecewise, continuous right hand sides. The program is suited to the simulation of systems with jumps in the state variables, the state derivatives, and in the controls.

The group has developed several techniques for the optimization of parameterized control functions with cost functions subject to differential, state, and boundary constraints. The condition number in multiple shooting methods has been improved through a new code – BDSCO – developed with the cooperation of the Technical University of Munich. The missile simulation code is called MISI.

Recent applications of the optimization codes have been directed at mission and trajectory planning in air-combat scenarios (Grimm and Well, 1987; Moritz et al., 1987). In these papers a new algorithm for differential games has been applied to developed guidance laws for medium-range air combat with missiles. The calculations indicate that optimal and suboptimal maneuvers orient themselves towards the boundaries of the flight envelope rather than towards energy climb paths.

Another area of investigation which has definite military applications involved a study on a guidance and control system for an intelligent munition (Kramer and Well, 1987). Kramer examines the active control of a gun-launched munition currently being developed in Germany. Bang-bang lateral thrusters are used to command angle of attack and thus generate lift. The reported control system has been used in a test firing of the actual munition, and further reports on the system are forthcoming.

Control

Dr. J. Ackermann described the work going on in the control group. The object of the group is to solve complex control problems through advanced control concepts, computer aided design procedures, and numerically reliable software. IDF considers software to be a method of transferring know-how to industrial and university units, thus the emphasis on software development at IDF. There are several programs available with RASP – a program library developed in cooperation with the University of Bochum – being of prime importance. The code is used for analysis, synthesis, and optimization in control systems. About 50 industrial, university, and research units use the code at present. Ackermann indicated that transfer of the code was treated in a fairly formal manner in that discussions were held with the

requesting institution as to their computer needs and how RASP might fit into their effort. He felt that this approach facilitated know-how transfer. As part of the transfer program there is a 3-year program for young engineers (supported 50 percent by industry and 50 percent by DFVLR) who work at DFVLR, using the software on industrial applications. As these engineers move into industrial employment they take their expertise in RASP and other software programs with them. Among the other software programs are REMVG, which permits systematic design of vector value performance indexes and parametric optimization. These designs are characterized by a variety of design specifications and technical realization constraints, a physical example of which might be a strongly cross-coupled system such as a helicopter. Work is currently being done on the development of ANDEC, a code which involves the application of artificial intelligence to control design.

Under the heading of "advanced control concepts" particular emphasis is directed at concepts of robustness where one has variations in the parameters of a known design or component failure and at adaptive control where one has component tuning for systems in which parameters are unknown. A recent robust design was that created for the Swedish aircraft Saab-Jas 39. A robust pitch damper for a command augmentation system based directly on flying qualities was designed with a large operating range without gain scheduling and using only pitch rate gyros as sensors. In another recent project (Steinhauser, 1987) a control system for a cryogenic wind tunnel was designed. The cryogenic wind tunnel was modeled as a nonlinear multi-input multi-output (MIMO) system with state-dependent time delays. Using model reduction and linearization, Steinhauser obtained a simplified model. For the simplified model he obtained the first controller design by pole placement. This controller was used as the initial system in a further optimization using a vector-valued performance index. The system is now in use in a DFVLR cryogenic wind tunnel at Cologne. A further example of the problems addressed by the control group is concerned with a multi-criteria control design for a preview vehicle-suspension system (Foag and Gruebel, 1987). Optimization of the design is based, as in the previously described system, on a vector performance index. The paper also illustrated the feasibility of previewing the road profile as a method for improving the performance of an active suspension system.

Ackermann's recent paper (Ackermann and Muench, 1987) on robust analysis in a plant parameter plane is an example of the computer aided design procedures developed at IDF. The analysis is based on the assumption that a linear plant model depends on two uncertain parameters, a and b , in an operating range $(a,b) \in \Omega$. In the frequency domain a given pole region is

specified based on bandwidth and time response in the normal manner. Rather than doing the robustness or further optimization of the design in the frequency domain the analysis is conducted in the parameter plane (a,b) by mapping the pole region into the parameter domain. If the coefficients of the characteristic polynomial are linear in the plant parameter the mapping is fairly simple. The design in the parameter plane is facilitated by graphics software and by the use of the IDF sensor ball (see below) which permits the interactive simultaneous variation of six system feedback gains or other constants of the system. Two detailed examples are given in the paper to illustrate the approach.

Automation

Dr. G. Hirzinger indicated that his group has been working for more than 10 years on the development of sensor and sensor feedback for robots. An excellent review of the work at IDF and indeed of the state of the art is given in a recent survey paper on sensory feedback in robotics (Hirzinger, 1987a). Among the equipment developed at IDF and used in the robotics laboratory are small force-torque sensors and optical range finders for end effectors. Hirzinger described two new sensors developed at IDF — one based on strain gauges arranged in a double maltese cross geometry and the other a compliance, optical, six-axis force torque sensor. The optical range sensor designed for a distance of 5-50 cm is shorter than a match stick.

A carefully designed man/machine interface consists of the IDF steering or sensor ball which permits the operator to position a robot arm arbitrarily. The sensor ball contains the optical compliance sensor and thus is capable of six degrees of freedom based on the forces and torques exerted by the human operator. A sophisticated three-dimensional computer graphics work station permits the operator to see the results of his inputs to the robot. A further advantage of the graphics presentation is being considered in an application to space and telerobotics (Hirzinger, 1987 b). The concept involves the use in a space laboratory mission of a robot which is capable of automatic learning of tasks and which can be either preprogrammed or operated remotely (teleoperation) from the ground. Since there is a built-in time delay between the commanded task and the motion of the robot the graphics system first shows the the result of the com-

mand and later the actual motion of the robot. This prevents overcompensation on the part of the human operator. I found a demonstration of the system to be quite impressive.

Conclusion

IDF is one of the best laboratories that I have visited in the controls area. The personnel are highly qualified and many of them have spent time working or studying in the US. The laboratory has a well-integrated series of software for the control and simulation of complex systems. The parameter plane method with supporting software is an excellent design method. Finally, the robotics laboratory sensor developments are very impressive and, I believe, represent the way that future advances in robotics will come about.

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FLUID MECHANICS

Fluid Mechanics at the Netherlands' National Aerospace Laboratory

by Daniel J. Collins. Dr. Collins is the Liaison Scientist for Aeronautics in Europe and the Middle East for the Office of Naval Research's London Branch Office. He is on leave until June 1988 from the Naval Postgraduate School where he is a Professor of Aeronautical Engineering.

The National Aerospace Laboratory (NLR), located in Amsterdam and Noordoostpolder, is the central aerospace organization of the Netherlands (see ESN 40-7:230-235 [1986] for previous NLR report, which emphasized numerical methods). NLR, with a budget of over 100 million guilders (\$58.8 million), has a staff of 800, about two-thirds of whom are university or technical college graduates. About 30 percent of the budget, funded directly by the Dutch government, is called "foundation support" while the remaining 70 percent is obtained from contracts, principally with the government. In 1986, 209 reports were prepared by NLR; of this number 131 were released for external distribution. Many of these reports are duplicates of conference presentations and papers presented in English or American journals.

The laboratory is divided into five operating divisions: Fluid Dynamics, Flight, Structures and Materials, Space, and Informatics. My visit to NLR was confined to the Fluid Mechanics Division, which is directed by Professor J. W. Slooff. Slooff, who gained some fame from his original analysis of the winged keel of the America Cup yachts (Slooff, 1985), has a joint appointment in the Aerospace Department of the University of Delft. The activities of the Fluid Mechanics Division are split between Amsterdam and the Noordoostpolder, where the larger windtunnels of NLR and the German-Dutch Wind Tunnel (DNW), run partly by personnel from NLR, are located. The Fluid Mechanics Division has a staff of 126 (86 professionals) and another 41 people involved with the running of DNW. Most activities at NLR are executed in project groups which cross division and departmental lines—the so-called matrix structure. The Fluid Mechanics Division has three main classes of activities: development support for industry (primarily involving wind tunnel testing), facilities-oriented research, and aircraft-oriented research.

The aircraft-oriented research is mainly connected with fixed-wing commercial transport. Recent strong emphasis has been on the Fokker 50 and Fokker 100 aircraft. The Fokker company depends on NLR for its theoretical aerodynamics support, and its aerodynamic testing is done at NLR under contract.

The division is divided into six departments:

- Incompressible aerodynamics
- Compressible aerodynamics
- Propulsion/acoustics aerodynamics
- Aeroelasticity
- Theoretical aerodynamics
- Wind tunnel instrumentation.

I shall review the activities of the first five departments, with emphasis on computational fluid dynamics (CFD) at NLR. The division operates several wind tunnel facilities which I will discuss along with each of the departments as I believe that gives a better description of the integration of activities of the entire division.

Incompressible Aerodynamics

Part of the activity of the incompressible or low-speed aerodynamics department (22 people), headed by Dr. B. van den Berg, is wind tunnel testing for industry. Recent aeronautical testing has concerned the Fokker 50, CN 235, Gulfstream, and aircraft for France's Bréguet-Dassault Company. The Fokker 50 tests were on the engine intake duct using a full-scale model of a part of the nacelle in the low-speed wind tunnel (LST) (3 m wide, 2.25 m high, 8.75 m long) with the purpose of improving the aerodynamic efficiency of the cooler. Demonstration measurements have recently been made by means of laser Doppler anemometry of the velocity field in the slipstream and between the blades of a model six-blade propeller for the Fokker 50 in the LST.

The wind tunnel, constructed in 1983, is atmospheric with a closed circuit and a maximum speed of 85 m/sec. Three interchangeable test sections permit two and three-dimensional (2-D and 3-D) tests to be conducted. Tests for industry include those for ships and offshore structures (with particular reference to helicopter operations) and the aerodynamics of buildings.

Further extensive work is done in the DNW, which is the largest low-speed wind tunnel of its kind in Europe. DNW has three interchangeable, closed test sections of 9.5x9.5x9.5 m, 8x6x6 m, and 6x6x6 m with corresponding velocities of 0-62 m/sec, 0-117 m/sec, and 0-153 m/sec. One of the unique features of the facility is the large anechoic chamber associated with the open test section

of the tunnel which is used in full-scale noise tests. Helicopter rotor noise has been measured, for example, in the open jet test section. Other tests that have been made in the DNW are a wind converter of the Darrieus type, a model Fokker 50 with propellers, and an Airbus model equipped with two turbine-powered simulators. The DNW is also equipped with a moving belt which permits accurate ground simulation of surface vehicle aerodynamics. It is difficult to realize the size of the tunnel if one has not seen it, but some idea of the size may be obtained when it is realized that full-scale testing of large trucks is done in the test chamber. A 1/10-scale model of the DNW is used by the Fluid Mechanics Division for research purposes.

Research activities in incompressible aerodynamics are directed at high-lift devices, boundary layers, and wind energy conversion. A recent paper in this area has been on the computation of 3-D boundary layer transition and separation on a 65-deg swept delta wing at 20-deg angle of attack (de Bruin and Hoeijmakers, 1986). Simple transition criteria were used for streamwise instability, cross-flow instability, and leading edge contamination. Comparison of experiment and theoretical pressure distributions showed that modeling of the secondary separation by means of a free vortex sheet improved agreement, but the predicted sharp suction peak underneath the secondary vortex was not found in the experiment. Several computer codes (VORSBA, BOLA, etc.) were used in the calculations. (These codes are mentioned below under theoretical aerodynamics.)

Compressible Aerodynamics

The Compressible (or high-speed) Aerodynamics Department (45 people) also does extensive wind tunnel testing for the aerospace industry. This includes, for civil aircraft, tests on the Airbus 300/310 and the Concorde as well as tests for Fokker, Bréguet-Dassault, and Messerschmitt-Bölkow-Blohm (MBB). Military testing has been done for Saab, MRCA, and Dassault among others. The high-speed tunnel (HST) is 2 m wide by 1.6 m high with an operating range of Mach 0 to 1.25. It is a continuous pressurized tunnel which is used for full, half, and 2-D models with blown nacelles and TPS. The tunnel has recently been used, along with the LST, in a series of extensive and detailed measurements on 2-D wing/flap configurations at various Reynolds and Mach numbers. These measurements have been part of a collaborative effort involving the Group for Aeronautical Research and Technology in Europe (GARTEUR). Work for other laboratories has included measurements of 2-D models to full Reynolds number, measurements of a half-span model of a wing with the same flaps, and flight testing. Other recent work has been concerned with the testing of the Fokker 100.

The department's supersonic tunnel (SST) is a blow-down facility with a cross section of 1.2×1.2 m and a Mach number range from 1.2 to 4. Models of the Ariane 3 have been tested in the tunnel. Two smaller tunnels are also available for research.

The department's research activities in compressible aerodynamics are directed at the study of transonic airfoils and wings, scale effects, shock-wave/boundary-layer interaction, code validation work, wall and support interference, and testing techniques. Recent reports in this area have considered 2-D wall interference effects in transonic flows and Reynolds number effects in the wind tunnel environment.

Propulsion/Acoustics Aerodynamics

There are two main areas of activity of the Propulsion and Acoustics Department (14 people), which is headed by Mr. J.W. Kooi. In the first activity connected with propulsion aerodynamics, the department supports engine simulation in wind tunnel tests, calibration of model engines, and thrust-minus-drag bookkeeping. In the second activity, connected with acoustics, the department supports acoustic measurements in the wind tunnel, develops and applies mathematical models for noise generation and propagation, and engages in acoustic linear research.

Engine simulation tests have been conducted for a variety of civilian and military aircraft as well as for air-breathing missiles in the NLR wind tunnels. Recent work has included thrust reverser experiments for the Gulfstream IV and the Fokker 100 aircraft and exhaust nozzle testing for the Fokker 50 with propeller. As part of the engine flow simulation techniques NLR has blown nacelles with hot and cold gas. In the turbopowered simulator (TPS) one has simulation of the inlet and the jet flow simultaneously. This technique, based on a modified Boeing design, uses H_2O_2 gas.

For study of jet noise the department has a small anechoic wind tunnel; acoustic linear testing is done in a duct flow facility. Acoustic measurements have been made on the six-bladed Fokker 50 propeller in the HST and in the DNW tunnels. Further studies have been made of noise transmission through fuselage panel walls, and in another experiment measurements were made of the noise field of fan noise produced by the interaction of the rotor and the stator blades in a through-flow nozzle.

Aeroelasticity

The Aeroelasticity Department (10 people), headed by Professor R.J. Zwaan, has four areas of activity involving unsteady aerodynamics, vibrations, flutter clearance, and active controls. The department makes unsteady pressure measurements on oscillating wind tunnel models; it also develops and applies computer codes in unsteady aerodynamics. Recent tests in this area in the

LST were on a wing model with a strake configuration and with partially sharp and strongly swept leading edges. Part of the test facilities are test rigs for such models. In the field of testing, the department conducts ground vibration tests and flutter clearance tests.

NLR has developed a code—ARSPNSC—for calculation of aerodynamic loads on oscillating, lifting, and nonlifting bodies in compressible uniform flow which has successfully been applied in subsonic flow (ESN 41-10:592-594 [1987]). Extension to this code are now in progress to supersonic flows with wings at high angle of attack with vortices. Two other codes, TULIPS and FTRANC, are being used in the study of transonic, oscillating 2-D airfoils. Comparisons between the two codes for standard configurations are being made. Experiments with supercritical airfoils which are undergoing buzz-phenomena are also being used in the validation of a new code, FTRAN2-NLR, which is applicable to transonic flows with boundary layers.

The application of active control for flutter suppression and gust alleviation has been another project done under the auspices of GARTEUR. In the final phase of this project spoilers were studied as control surfaces (Foersching, ed., 1986)

Theoretical Aerodynamics

The Theoretical Aerodynamics Department (10 people), headed by Dr. B. Oskram, is concerned with the development, validation, and application of computational fluid mechanics (CFD) codes or tools to be applied in aircraft analysis and design. The department is supported by an additional 10 to 15 people in the Informatics Division in mathematical modeling, numerical analysis, and programming.

Department personnel have developed computer codes (about 24) in the following areas: Euler, full-potential, panel methods, vortex flow, boundary-layers, design, and propeller aerodynamics. I will make some comments on the codes for each of these areas and give current references.

Euler. Practical problems under Euler code analysis are concerned with wing/nacelle interaction, transonic flows, highly swept wing configurations, and canard-wing interactions. Most of these codes are based on FLO57, by Jameson. A major problem in CFD calculations of complex configurations such as those with propeller slipstream and exhaust gases is the grid generation process. The NLR solution to this problem is reported by Boerstoeel (1986a).

Full Potential. Perhaps the principal code in this area is MATRICS (van der Vooren et al., 1986), which is a finite volume, fast solver, for general 3-D civil aircraft configurations. Part of the development of this code, particularly the grid generation part, has been in cooperation

with the Aeronautical Research Institute (FFA) of Sweden. Validation calculation for transonic flow over transport aircraft are given by Van der Vooren both with and without propeller influence. There is also a 2-D finite volume code, TRAFS, for transonic airfoil calculations and (for the fuselage) a code, XFLO22, for cross-plane calculation which is in heavy use.

Panel Methods. Two codes using advanced high-order panel methods with application to 3-D complex geometries, wakes, and lifting surfaces are under development (AEROPAN and PDAERO). A code that has been used extensively is "NLR Panel Method." It is this code that has been extended to hydrodynamic flows around ships with free surface effects (Van Beek et al., 1985). A subsonic and supersonic panel code for complex geometries—NLRAERO—has been transferred to the Naval Weapons Center at China Lake, where it is presently being used.

Vortex Flow. NLR has a strong program in the study of vortex flows, as witnessed by the recent lectures presented by Hoeijmakers (1986) at the Von Karman Institute for Fluid Mechanics (ESN 41-10:563-566 [1987]). These lecture notes not only give an excellent tutorial on the strength and weakness of vortex flow calculations but also give a detailed discussion of the codes developed and used at NLR in this area (VOR2DT, VORSBA, VORSEP). Detailed calculations are given of each of the codes (delta wings, slender bodies, vortex separations, etc.) with comparisons from other calculations. Both code and experimental comparisons indicate that NLR has developed and uses very sophisticated, state-of-the-art numerical codes.

Boundary Layers, Design, and Propellers. Application of boundary layer codes has already been discussed with respect to experiments on high-angle-of-attack delta wings (de Bruin and Hoeijmakers, 1986). Design methods are directed at computer aided design (CAD), particularly of multielement airfoils. My impression was that the purchase of a new computer work station (Sun) would put more emphasis on this area in the future. There are two codes available for the analysis of propellers in axial flow.

Conclusion

NLR is a center of excellence in CFD and fluid mechanics experimental research in the Netherlands and has good ties with academia. There is an appropriate balance between experimental and theoretical methods. The Theoretical Aerodynamics Department has produced some excellent computer codes dealing with Euler, potential, and vortex flows as well as with boundary layer analysis. The new supercomputer, identified below, should extend the Fluid Mechanics Division com-

petence into the application concerning the full Navier-Stokes equations.

I have 32 reports summarizing the CFD effort of NLR which I can make available to interested parties. One of the more interesting reports (Boerstoeel et al., 1986b) is an overall review of the CFD in the Netherlands. This report includes current developments and projected developments both in CFD and in the management and establishment of an engineering data base making readily available the CFD codes to engineers. One projected development is the application of the Navier-Stokes calculations to the description of aerodynamic flows. The Dutch effort in this area is just beginning through a national project involving not only NRL but Delft University and other Dutch institutions. The need for a supercomputer in 3-D Navier-Stokes calculations has been recognized in the recent purchase of a NEC SX-2. This computer will be added to the NLR computer network and was expected to be available for use in early 1988.

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11/30/87

MATERIAL SCIENCES

Fifth European Conference on Internal Friction and Ultrasonic Attenuation in Solids

by R.W. Judy. Dr. Judy is Superintendent of the Materials Sciences and Technology Division, Naval Research Laboratory, Washington, DC.

The fifth European Conference on Internal Friction and Ultrasonic Attenuation in Solids was held from 26 through 30 July 1987 at the Rijksuniversiteit Centrum of the University of Antwerp, Belgium. This conference series is intended primarily for those in the European science community involved in the field to meet on a 4-year schedule that alternates with the international conference series. The location and timing of the conference were selected to encourage the participation of students to the greatest extent possible. The format of the conference was the poster and rapporteur system for the contributed papers, with six invited lectures in selected topics. Additionally, an evening workshop on materials for high acoustic damping was included in the program. About 100 attendees were present, mostly from France, Switzerland, Belgium, and West Germany, although representatives from as far away as China and Argentina attended. There were six registered participants from the US. The conference chairman was Professor R. DeBatist

of the Study Center for Nuclear Energy (SCK), Mol (near Antwerp); he and his staff provided excellent accommodations and arrangements for the conference participants. Conference proceedings will be available later; contact Professor DeBatist to obtain a copy.

The Invited Lectures

Each of the six invited papers was allotted 1 hour for presentation and discussion. These were selected to be state-of-the-art papers in different aspects of internal friction and ultrasonic attenuation. The first was "Stress Relaxation in Solids," by J. Kubat and M. Righdahl, both from Chalmers University of Technology, Goteborg, Sweden. The authors presented a model describing the stress relaxation in any terms of three adjustable parameters: the internal stress, the relaxation time, and a parameter characterizing the shape of the relaxation curve. It was shown that the expression reproduces the

stress relaxation in metals, ceramics, and polymers. A lively discussion which followed the talk centered around the nature of the fully relaxed state.

The second paper, "Hysteretic Damping Mechanisms Related with Dislocation Motion," was presented by M. Gremaud of the Ecole Polytechnique Fédérale de Lausanne (Switzerland). Professor Gremaud presented a general phenomenological theory of internal friction. The theory makes it possible to identify the basic phenomenological process giving rise to internal friction by analyzing amplitude, temperature, and frequency dependence. He gave examples and showed, in particular, how one can attribute intermediate hysteretic damping in terms of the relaxation of the dislocations with respect to the Cottrell-cloud.

Dr. E.H. Brandt, Max Planck Institut für Metallforschung, Institut für Physik, Stuttgart, West Germany, presented "Flux-Line Pinning Effects in Superconducting Vibrating Reeds." He described very recent work on high T_c superconducting metallic materials and showed that the presence of a longitudinally applied magnetic field caused the resonant frequency and the damping capacity to increase dramatically—e.g., by factors of 500 and 10^5 , respectively. The resonance frequency increases because the vibrations of the reed tilt the flux lines periodically, which ultimately is equivalent to an additional surface tension. Linear and nonlinear damping result from the motion of pinned and depinned flux lines. Depinning occurs at amplitudes in excess of 30 A, and the enhancement of damping may be used to study this process.

The fourth invited paper, "Recent Progress of Investigations on Elastic and Anelastic Properties of Concentrated Metal-Hydrogen Systems," was presented by F.M. Mazzolai, of the University of Perugia, Italy. The thrust of the paper was the formation of metal hydrides and the mechanisms of stress relaxation they cause in Nb-V-H and Ti-V-H systems. The elastic constant was investigated at high frequencies near phase transitions in Nb-H(D) and showed that either softening or discontinuities occurred, according to the nature of the transition. One conclusion of the paper was that the Zener relaxation in FCC metals can be used to monitor short-range order in binary alloys.

Dr. D.P. Almond of the University of Bath, UK, presented an invited talk, "Ultrasonic Studies of Ionic Conductors." His paper described ultrasonic attenuation peaks at low temperatures in sodium-beta alumina, which is typical of ionic conductors for solid electrolytes in advanced batteries. Attenuation peaks, which are thermally activated, could be characterized by a power-law expression developed earlier by Jonscher for dielectric relaxation phenomena. Closely related expressions were fit to the high-frequency dispersion in the AC conductivity. A similar pattern of equivalent acoustic and

electrical characteristics was found in other ionic conductors, including ionically conducting glasses, which are quite unlike beta alumina. The ultrasonic studies facilitated an independent assessment of ionic hopping rate and thus they complement the electrical measurements. The studies emphasized the importance of the role of entropy of activation in determining the magnitude of the ionic conductivity in such conductors.

The final invited paper, presented by Professor A. Seeger of the Max-Planck Institut für Metallforschung, Institut für Physik, Stuttgart, was titled "A Physical Picture for the Internal Friction due to Dislocations and Atomic-Defect-Dislocation Interactions." The talk was essentially a review of the discontinuous theory of dislocation damping. Dr. Seeger stressed the important differences of this theory and the continuous model of Reed-Koehler-Granato-Lücke. The stochastic nature of the discontinuous theory can differentiate in much more detail between different elementary damping processes and, coupled with recent data, permits a much better understanding of the point defect-dislocation interactions.

The Contributed Papers and an Evening Workshop

The quality of the contributed papers was very high. These papers were organized into the topics of dislocations (two sessions, 24 papers), transformations and interfaces (two sessions, 35 papers), techniques and modeling (14 papers), and point defects (12 papers). An increasing number of contributions on questions associated with phase transformations, both diffusion-controlled and diffusionless, was generally noted. Another trend was set by the appearance of industrially motivated studies, such as the internal friction of quartz as a function of adsorbed or absorbed water. In each session, the rapporteur selected one paper for presentation by the author. The schedule was arranged to permit ample time following the rapporteur's presentation for viewing the posters, followed by a general discussion period. Discussions were quite lively at times, which indicates the high degree of interest in the papers. This phase of the conference had a rather relaxed, informal atmosphere that signified the spirit of collaboration among the participants, as opposed to the competitive environment I have often observed at other conferences.

An evening workshop on high damping materials was organized and chaired by Professor M. Wuttig of the University of Maryland (College Park), and Dr. J. Van Humbeeck of the Katholieke Universiteit Leuven, Belgium. The meeting was started by Professor Wuttig, wherein he presented a three-parameter description of damping and the interdependency of defect content and elastic properties (modulus) on specific damping capacity. This was followed by widely ranging discussions

of all aspects of acoustic damping and materials to achieve improved damping. Many participants were interested in the engineering aspects of problem solving, rather than in means for improving the damping properties of metallic materials. Several ingenious schemes for absorption of acoustic energy were presented and discussed.

Conclusion

The final activity of the meeting was to select a site for the next European Conference, to be held in 1991.

The place chosen is Cracow, Poland, with Dr. E. Klugmann of the Technical University of Gdansk to be the conference organizer. The International Conference on Internal Friction, which will take place in 1989, will be held in Beijing, China.

3/14/88

Wear Resistant Materials Meeting in France

by Louis Cartz. Dr. Cartz is the Liaison Scientist for Materials Science in Europe and the Middle East for the Office of Naval Research's London Branch Office. He is on leave until June 1988 from Marquette University, College of Engineering, Milwaukee, Wisconsin.

Introduction

A meeting titled "Surface Treatment of Wear Resistant Materials" was held from 18 through 20 November at the Centre d'Etudes des Métaux, Ecole Nationale Supérieure des Mines (ENSM), St. Etienne, France. It was organized by five French associations devoted respectively to metallurgy, ceramics, special steels, and heat treatment techniques. Though the meeting was announced as an "International Colloquium," the participants, about 100 in number, were almost entirely from France, with just one or two each from Belgium, Switzerland, Italy, West Germany, and Japan. While the majority of the papers were given in French, those of the Japanese and West Germans were in English. In any case, simultaneous translations were given in English and French. A useful set of extended abstracts was provided at the time of the meeting, with English translations where necessary.

The sessions were organized to cover:

- Thermal, chemical, and mechanical treatments
- Ion implantation of surfaces
- Hard coatings by vapor deposition
- Ceramic coatings.

The organizers do not plan to publish the proceedings of the meeting. A total of 22 papers were given, of which two were from West Germany and one from each of Japan, Switzerland, and Italy. About half of the papers were by speakers from the St. Etienne-Lyons region of France. In fact, five papers were presented by scientists from Unirec, Firminy (near St. Etienne). (A description of the Unirec research laboratory was given in *ESN* 41-5:271-273 [1987]). Unirec, incidentally, is now part of the Institut de Recherche de la Sidérurgie, France (IRSID),

which is the research institute supported by the steel producers of France.

This report is concerned in particular with the presentations on ion implantation techniques, vapor deposition, and thermal/laser treatment.

General Review of Wear

The conference was introduced by an excellent review by R. Leveque (Unirec, Firminy) of the different mechanisms of wear surface damage and of surface treatments to enhance wear resistance. This was the perfect way to begin the conference. Leveque described the wear processes of abrasion, adhesion, surface fatigue, contact corrosion, erosion, cavitation, chemical and electrochemical corrosion, and thermal fatigue. He also discussed the various surface treatments of structural transformations, thermochemical treatments, surface conversion, and coatings. Leveque summarized the wear processes as depending on physical chemical factors (chemical reactivity, atomic diffusion, oxidation), mechanical processes (topology, hardness, crack resistance, residual strains), and metallurgical aspects (crystal structure, proportion of hard phases, grain sizes, atmosphere, and temperature).

Surface Treatment by Ion Implantation

The wear resistance of steels is known to be improved by N implantation when nitrogen migration occurs during the wear process, though this is not understood. Iron implanted with Si forms an amorphous surface layer. D. Treheux (Ecole Centrale de Lyon, Ecully, France) has in-

vestigated these phenomena in several stainless steels using a range of surface studies including transmission electric microscopy (TEM) of thinned sections, grazing incidence x-ray diffraction (GIXD), Mossbauer spectroscopy, and Rutherford backscattering. Stainless steels (18 percent Cr, 10 percent Ni) have been implanted at a range of temperatures by a nitrogen fluence of 2×10^{17} ions/cm² at 40 keV. Iron has been implanted with Si at room temperature with 5×10^{16} to 2×10^{17} ion/cm² at 40 keV. The observations by TEM have shown that the nitrogen-implanted steel has a surface layer composed of highly oriented mixed nitrides (or carbonitrides) of $\epsilon\text{Fe}_2\text{N}$ and $\epsilon\text{Fe}_2(\text{N},\text{C})$. The implantation retards the oxidation of the worn surface layer, which resists wear and retains its hardness after many hours of use. Fine scratches of the surface layer induce crystallization of nitrides along the scratch path. Fracture of the outside layer appears to be due to austenite twinning of the substrate. High densities of dislocations and stacking faults quickly form in the worn surface layer. As surface wear progresses, a highly strained, hardened surface layer forms; it contains nitride precipitates (ppt) which have been pushed down during the wear process. This accounts for the observation of a nitrogen content deeper down into the surface than can be explained by the penetration power of the ion beam.

The silicon-implanted layer in iron is known to form an amorphous layer (at $\sim 10^{17}$ ions/cm²) containing ppt of Fe_3Si . Observations by TEM of wear surface regions show recrystallization of amorphous to an Fe-silicide, high densities of dislocations, and austenitic twinning. The role of the Si is to prevent abrasion and plastic flow by increasing the hardness, spreading the stresses over larger volumes of the substrate.

A. Pichat (Ecole Nationale Supérieure des Mines de St. Etienne) reported on wear tests on orthopedic prosthesis Ti-6Al-4V alloys implanted with N at 80 keV and 2×10^{17} ions/cm², used against a high-molecular-weight polyethylene. The wear characteristics are improved but there is a tendency for the wear surfaces to seize up. P. Mille (Ecole Nationale Supérieure des Arts et Industries de Strasbourg, France) also reported on ion implantation studies in Ti-6Al-4V of N at 40 keV and $2-4 \times 10^{17}$ ions/cm², for different implantation currents. Continuous processing of specimens is carried out using a moving belt with an ion scanning system to implant large surface areas. The specimens have been examined by TEM and electron diffraction studies, and by secondary ion mass spectroscopy (SIMS). The SIMS profiles of the depth of penetration of N into the Ti alloy were carried out using oxygen ions of energy 10 keV, giving rise to a sputtering rate of 720 nm/hour. By assuming a Gaussian distribution, the N-ranges are found to be about 70 nm and range distribution widths of about 40 nm. The Ti alloy has a small grain size, and the presence of TiN and α -Ti (grain sizes 30-50 nm) has been identified. Though

the implanted layer is a fraction of a micron deep, there is a marked improvement in fatigue properties. The implantations apparently give rise to a surface layer under compression, and when this corresponds to the yield stress, ion implantation has no further effect.

A. Belbach (Ecole Centrale de Lyon, Ecully, France) has studied the friction and wear characteristics of Co-cemented WC implanted with N (40 keV and 60 keV) as a function of several implantation parameters, cobalt content, and friction conditions. A rotating sphere against a flat plate tribometer was used and also a pin-on-disc tribometer. Examinations were carried out by TEM and GIXD. The effects of N-implantation were found to be as follows:

- The implantation does not change the friction coefficient.
- Oxidation products of Fe, W, and Co are less noticeable.
- Some positive, though sometimes some negative, effects on wear resulted which may have been caused by Al_2O_3 impurities.
- The cobalt appears to be "amorphised."

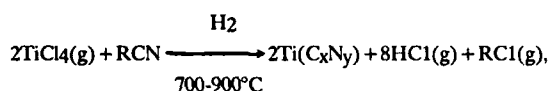
N-implantation of cemented carbides may result in beneficial wear properties though only in particular cases of Co content and of implantation conditions.

W. Lohman (ENKA AG, Obernburg, West Germany) described the application of ion beam mixing to form hard protective coatings. The method, which is intended to enhance the adhesion of the deposited layer, combines physical vapor deposition (PVD) and ion implantation. Experiments were carried out on TiN coatings, and on Al_2O_3 coatings. These coatings are first deposited by RF Magnetron sputtering. The TiN layer of thickness 90 nm was deposited on a Mo stainless steel. The ion beam mixing used Ar ions at 150 keV, of fluence 10^{16} ions/cm². Adhesion was measured by a scratch test up to a critical load, as detected by acoustic emission when film breakdown occurs. The Al_2O_3 film, thickness 100 nm, was similarly deposited on a tool steel. The Al_2O_3 layer had improved adhesion, while adhesion of the TiN layer was reduced. It is believed that compressive stresses are induced by the ion implantation for Al_2O_3 , resulting in improved adhesion, and that this is not the case for the TiN layer. However, measurements have not been made of the induced stresses in the surface layers.

Surface Treatment by Vapor Deposition

Chemical Vapor Deposition (CVD) methods of depositing hard antiwear coatings were reviewed by R. Bonetti (Berna AG Olten, Switzerland). He gave the ex-

ample of the deposition of Ti carbonitride, for which the reaction is



where R is an organic radical. The reaction at the solid-gas heterogeneous interface gives rise to a dense deposit.

The wear-resistance properties of Cr carbide and of Cr nitride coatings deposited by CVD were discussed by J.F. Nowak (Unirec, Firminy, France). The Cr nitride deposit on stainless steel (SS) is obtained by N₂ ion bombardment of the SS surface, followed by Cr vapor at 900-1000°C. A compact, uniform layer of thickness about 25 μm is obtained of Cr₂N, and the SS substrate contains a dispersion of a fine ppt of nitride. The Cr/N ratio is constant throughout the deposit, decreasing near the SS metal interface. The βCr₂N crystals have a planar hexagonal structure and the basal planes tend to be parallel to the metal surface. The Cr carbide coating is formed at low pressure by the pyrolysis in a hot-wall reactor of Cr dicumene. The structure of the coating depends on the pyrolysis temperature (600°C maximum) and on the organometallic precursor used. Coatings formed between 325 and 450°C are amorphous, inhomogeneous in C composition; coatings formed between 450 and 500°C are amorphous but with composition corresponding to Cr₇C₃. Above 500°C, coatings form with highly crystalline-oriented Cr₇C₃, with the highest hardness factor. Both types of coatings, Cr₂N and Cr₇C₃, are highly resistant to abrasion, and resistant to corrosion by sulfuric acid, phosphates, seawater, and corrosive liquids. The coatings are harder in the crystalline state than in the amorphous state.

J.P. Terrat (Hydromécanique et Frottement, Andrezieux-Boutheon, France) reported on a wide-ranging study of the microstructure and properties of surface coatings deposited by magnetron sputtering (PVD). He related the deposition conditions of substrate temperature and deposition rate to microstructure texture, micro- and macroresidual stresses, Knoop hardness, and rubbing tribometry for coatings of several nitrides of Cu, Al, Mo, Cr, Ti, and (Fe, Ni, Cr) alloys. Pole figures of the

crystal structure orientations were determined using x-ray diffraction methods. The residual macrostresses were determined from the lattice parameter measurements of the compounds, and the x-ray peak widths give a measure of the local variation in the residual stresses – the microstresses.

The nitride coatings studied were of Cr, Fe, Ti, and Mo – which give hard coatings – and of Cu and Al nitrides for their electrical properties. These nitrides have a range of m.p. from 933 K to 2890 K. There is interest in the fact that the concentration of N in the coatings is known in some cases to exceed the thermodynamic equilibrium values. All of the coatings are highly textured, with distinct preferred orientations similar to those found in bulk specimens. The coatings were all carried out on steel plates, precleaned by Ar ion bombardment, in a vacuum of 2x10⁻⁹ bar, substrate temperatures below 400°C, at 25 μm/hour, to a thickness of 10 μm.

The residual stresses and phases observed are summarized in Table I, where TS is the m.p. of the coating and TF the temperatures of the substrate during the coating. The changes in the microstresses can be related to the thermal mismatch between the coating and substrate; compressive residual microstresses are observed for those coatings having a thermal expansion coefficient lower than that of Fe (the substrate), and vice versa. The N content also plays a role; the residual macrostresses increase with N as shown in Figure 1, the effect increasing with the m.p. of the coating metal. The parameter η in Figure 1 gives the N saturation level, where η = 1 corresponds to the N-concentration of the solid solution at which point the nitride would form. The microhardness of Mo and Cr attain a maximum for η = 1.

Coatings by Thermal And Plasma Spray

Y. Matsubara (Kurume College of Technology, Kurume-shi, Japan) presented results of his examination of Cr-W-B coatings sprayed onto Co substrates. At the interface of the coating/substrate he observed a diffusion zone of an alloyed region. The adhesion of the coating to the substrate is dependent on the width, W(A), of the diffusion alloyed zone. The widths, W(A), are found to vary

Table 1. Crystal Phases, texture and stresses in nitride coatings, determined by X-ray methods. Ts is the m.p. of the coating Tf is the substrate temperature during coating..

Nature of Deposit	Phases after N ₂ Saturation	Texture Analysis		Hydrostatic Stress (Macro)	Residual Stress (Micro)	TS/ TF
		Fiber Components	Sharpness			
Al	AlN	<111>, <110>	s	tensile	tensile	0.5
Cu	no saturation	<100>	w	tensile	tensile	0.37
Fe	Fe ₄ N, Fe ₂ N	<100>, <110>	vs	tensile	tensile or compressive	0.29
Cr	β-Cr ₂ N	<111>, <100>	ms	tensile	compressive	0.22
Mo	γ-Mo ₂ N	<110>	vs	tensile	compressive	0.16

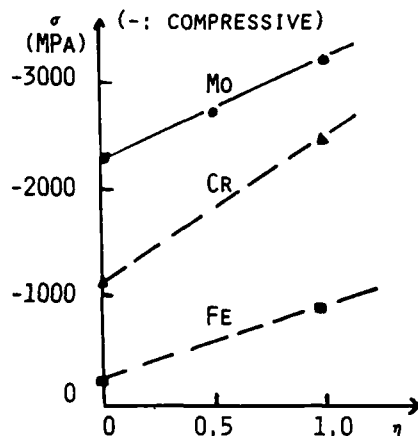


Figure 1. Macrostresses (σ) versus nitrogen content (η). The parameter $\eta = 1$ corresponds to nitrogen concentration for the nitride to form.

with temperature and length of time, t , of the diffusion treatment, when it is found that $W(A)^2 = kt$. The variation of k with temperature T follows an exponential law, $k = k_0 \exp(-Q/RT)$, where Q is an activation energy, which is found to be 87 kcal/mol. This value is comparable to the activation energies of diffusion of Co, Cr, and Ni in γ -Fe. Analysis by electron microprobe analysis of the diffusion zone gives a composition indicating that both substrate and coating have diffused into the zone, giving rise to the bond between coating and substrate. From the compositions of the diffusion zone, Matsubara considered that crystals present are likely to be cobalt and chromium borides with a W boride containing Co and Cr. He considers the matrix to be a solid solution of Co and Cr with some Ni and Si.

A. Boucher (Unirec, Firminy, France) described a coating process combining the advantages of plasma spraying and of plasma-transferred arc welding. The sprayed powders are preheated during their transport to the substrate by introducing the particles into a blown arc. The electric arc heats the surface further to weld the particles to the substrate.

Surface Treatment by Laser Heating

The treatment of surface by lasers to improve wear resistance by increasing toughness and surface hardness was reviewed by D. Burchards (Institut für Werkstoffkunde und Werkstofftechnik, Clausthal, West Germany). The treatment can be by transformation hardening, by surface melting, by surface alloying, or by cladding. The surfaces can be heated by high-power CO_2 lasers (10^5 W cm^{-2}), heating the surfaces very rapidly with a scanning mechanism, and achieving rapid cooling rates of 10^4 to 10^7 K s^{-1} .

Transformation hardening is of interest for the medium carbon steels and cast Fe; on heating, austenite

is formed which on quenching transforms to martensite. There can be selective hardening of critical parts of the specimen's surface, with minimum heat affected zones, avoiding ferrite formation. The case depth is typically 0.2 to 1.0 mm. Examples are laser-hardened teeth of gearwheels, when just the tips are treated to give the highest hardness values, and similarly for diesel engine cylinder liners. It is not necessary to treat the whole component, just the surface; the nonhardened region acts as a lubricant and can absorb damage.

Surface melting by laser heating is of interest for cast Fe when the rapid cooling gives rise to ledeburite formation; the surface hardness is increased and the wear properties are improved. Surface melting by laser heating is found to be a better treatment than tungsten inert gas (TIG) melting procedures because it results in a finer microstructure.

Surface alloying can be carried out using a gas or a solid. An example of surface-gas alloying is in the use of N_2 gas with Ti metal to form TiN at the surface. This is a very important method of improving the surface properties of Ti. Relatively large amounts of N are absorbed by Ti, forming a Ti-nitride which is stable over a wide range of compositions. The resulting surface is smooth, and the dimensions of the specimen are not altered appreciably.

An example of surface alloying with solids is the addition of Cr to a specific area of cast Fe; this is a less expensive method of material cladding. The surface layer is a Cr-rich ledeburite which is corrosion and wear resistant. Hard metal coatings, for example with WC powders, are formed by plasma spraying followed by laser heating in a protective atmosphere; the heating needs to be carefully controlled to avoid melting too much substrate, thus achieving better control of composition. Pores are removed and a fine crystalline texture structure is formed. This process has been used by Rolls-Royce to treat the leading edge of turbine blades.

P. Antona (Centre de recherches FIAT, Orbassano, Italy) reviewed laser hardening of cast Fe and Al alloys. The working rate is important since if the cooling is too rapid, not everything goes into solution, resulting in nonuniform surface compositions, which leads to possible nonuniform residual stresses. The rate of cooling can be modified by preheating the specimen. There is the problem of porosity which may be left behind in the sub-surface.

Other Treatments

The effect of controlled impact prestressing (shot peening) on wear characteristics was discussed by P.A. Dawson (Metal Improvement Co., Bayonne, France). The shot, propelled by compressed air at $\sim 120 \text{ ms}^{-1}$, causes deformation with plastic flow, leaving residual stresses, with damage depths of $\sim 1 \text{ mm}$. The variables

are energy of the jet of shot, the shape of the shot, and the hardness of shot relative to that of the target. Scanning (peenscan) can make the treatment more uniform over a surface. Dawson discussed the increase in surface hardness and how this may be used to improve wear resistance.

O. Longeot (Ecole Nationale Supérieure d'Arts et Métiers, Talence, France) described surface tempering by induction heating, followed by water quenching. Maximum temperatures are about 1500 K, quenching in < 8 s, with thermal cooling of up to ~ 300 Ks⁻¹. Phase transformations in steel can be induced depending on the steel composition and cooling conditions. Longeot has set up a model to calculate surface microhardness versus quench rates.

Comments

This conference was well organized, with very good provision for translating the presentations into English,

and also with the English-translated extended abstracts, available at the time of the meeting. Several good review papers were presented (Leveque on mechanism of wear surface damage and surface treatments; Treheux on ion implantation in Fe; Burchard on laser surface treatments). Approximately one-half of the papers came from industry and one-half from research institutes and universities in France, which, incidentally, cooperate well together.

Most significant are the results obtained by Treheux on N-implantation of steels. The hardened surface layer formed persists over greater depths than can be explained by the penetration of the nitrogen. Treheux has shown that as the surface wears down, hard ppt of Fe nitrides and Fe carbonitides are pushed down during the wear process. This observation is very important and is worthy of further study.

12/30/87

Engineering Ceramics at the European Joint Research Center at Petten, The Netherlands

Louis Cartz

Introduction

This report concerns the high-temperature materials studies, particularly on the stability of materials in severe environments, which are carried out at the European Joint Research Center (JRC) at Petten, the Netherlands.

The Petten Center is one of four JRC's (one each in Belgium, Italy, West Germany, and the Netherlands) whose research in engineering ceramics is supported by the Commission for the European Communities (CEC). This support is purposed to reinforce the individual national efforts, and also to stimulate collaboration across national boundaries and between industries, universities, and research institutes. The CEC organizes research programs for ceramics as shared-cost joint programs at universities and research organizations as well as at the JRC's; some of these programs are shown in Table 1.

The Petten Center, like the other three, has a multinational staff corresponding to the CEC populations. Petten's total staff numbers about 200 persons, of whom approximately 55 work in the High-Temperature Materials Department, which is headed by M.H. van de Voorde.

Ceramic Research at the Petten Center

Petten's high-temperature research program, begun in 1976, was concerned with metallic alloys and coatings, but was extended in 1984 to include high-temperature engineering ceramics. The studies are particularly concerned with the deterioration mechanisms of materials under severe environments of combinations of high temperatures, corrosive atmospheres, and mechanical stresses. Future studies are planned on metal ceramic joining, and on the surface modification of materials by implantation and by ion bombardment. The corrosion

Table 1. Some CEC research programs.

STIMULATION (1985-1987): Fundamental Studies of the physics and chemistry of surfaces.
EURAM (1983-1985): Material Development, including processing of the monolithic ceramics SiC, Si ₃ N ₄ , ZrO ₂ , Al ₂ O ₃ ; whisker/fibre composites, transformation toughening, surface coatings, non-destructive testing.
BRITE (1985-1989): Industrial Research of Cutting tool development, Laser technologies, Joining techniques, Powder production, Composites processing. Some of the CEC Programs of Ceramics Research and Development.

studies on metal alloys are carried out by J.F. Norton and J.B. Marriott, the corrosive studies on ceramics by R.J. Fordham, ceramic processing by D. McGarry, and powder characterization by A. Pizzolo, along with other workers.

High-Temperature Corrosive Problems. The corrosion studies at JCR Petten have been very carefully related to realistic industrial problems, such as those listed in Table 2 (see van der Voorde, 1987). The corrosion reactions studied are gaseous reacting species (O_2 , oxides of carbon, S and N, H_2 , H_2S) and metallic impurities (alkali salts and metal oxides, particularly V_2O_5). Because of the nature of the gases used these studies are conducted in a specially built laboratory in which autoclaves ($1500^\circ C$), thermobalances, and creep rigs ($1050^\circ C$) are available.

Corrosion of Si_3N_4 at High Temperature. JRC Petten is conducting an extensive research study on Si_3N_4 which is being supported by work in three other countries. The overall program is concerned with the relationship between processing, microstructure, and behavior under severe environments, as related to industrial conditions of usage.

Petten prepares the Si_3N_4 ceramics, using powder from Feldmühle, Stuttgart, by a range of methods:

- Sintered Si_3N_4 SSN with additives (Y_2O_3 , 9 percent, MgO , 1.5 percent; ZrO_2 in future work) at $1800^\circ C$, under ~ 100 -bar pressure of N_2
- Sintered reaction-bonded Si_3N_4 (SRBSN) (metallic Si powder with sintering aids is compressed into shape and nitrated at $1400^\circ C$, then sintered or hot pressed at $1700^\circ C$)
- Hot-pressed Si_3N_4 (HPSN) (1-5 percent additives, 50 MPa, $1700^\circ C$).

The mechanical properties being determined by Petten are:

- Strength in air, up to $1450^\circ C$, by four-point bending
- Creep in vacuum, air, and corrosive atmospheres, at temperature from 1200 to $1450^\circ C$, by four-point bending and tension studies
- Fatigue measurement in air, vacuum, and corrosive atmospheres, at temperature from 800 to $1400^\circ C$, measuring bending stress rupture and crack growth, using static and cyclic loads.

The support studies for this program are:

- Oxidation of Si_3N_4 in air (M. Billy and Mme. M. Desmaison, University of Limoges, France)
- Corrosion of Si_3N_4 in Na_2SO_4 and V_2O_5 studies (F. Riley, University of Leeds, UK)

Behavior of Si_3N_4 Ceramic. The Si_3N_4 powder characteristics measured by the Petten investigators are: average particle sizes, measured by sedigraph (ethanol dispersion); surface area, measured by BET absorption methods; inorganic impurities content; and surface characteristics, analyzed by electron optical and spectroscopic methods. The microstructures developed in the Si_3N_4 ceramic are followed with the time and temperature of the sintering process. The electron microscopic studies are used to reveal the different phases present—for example, βSi_3N_4 and N-melilite are often found surrounded by the original αSi_3N_4 grains.

Corrosion in O, C/O and S/O Atmospheres. The effects of corrosion of Si_3N_4 ceramic in oxygen, in C/O, and in S/O have been studied (see Fordham et al., 1987). At $1000^\circ C$ in air, there is a rapid weight increase parabolic with time, followed by a weight loss, which is not yet understood. Blow holes are frequently observed. This is being studied for different amounts of Y_2O_3 additives in the presence of other oxides. Experiments have been carried out in carbonizing-oxidizing atmospheres at $1050^\circ C$ and $1300^\circ C$ with partial pressures of oxygen from 10^{-27} bar to 10^{-20} bar, measuring weight changes for periods up

Table 2. Some industrial high-temperature corrosion problems.

	Components	Maximum Temperatures ($^\circ C$)	Environment and Corrosion Mechanism
Chlorinated organic compounds	Pyrolysis furnace tubes	825	Halides
Carbon regeneration	Grids	980	Oxidation, carburization
Phosphorus production	Reactor internals	820	Reactions with P_2O_5
Ethylene cracking and steam reforming	Pyrolysis tubes	1100	Oxidation, carburization
Petroleum coke calcining	Recuperators	870	Sulphur sand sulphides
Waste incineration boilers	Internals, super heater tube	980	Flue gas with salts, S, Zn, Pb
Pulp and paper recovery boilers	Smelt spouts	930	Molten salt attack
Aluminum remelting	Recuperators	1200	Flue gas with salts, halogen, S
Steel forgings	Recuperators	1200	Oxidation
Steel reheating	Recuperators	1200	Fuel ash corrosion
Mineral calcining	Calciners	1200	Oxidation, Sulphidation, halides
Si, SiO_2 and TiO_2	Reactors vessel	540	Halides
Pottery Kilns	Kiln components	1200	Oxidation
Gas carburizing	Furnace components	1100	Carburization
Fiberglass production	Recuperators	1200	Flue gas with salts, alkali metals, sulphur

to 250 hours. X-ray and electron diffraction studies show the presence of SiC needle-like crystals, attached at one end to a minute sphere, rich in iron. Studies have also been carried out in CO/H₂, CH₄/H₂O/H₂, and H₂/H₂S atmospheres, when there is a marked temperature dependence. Corrosive studies have been carried out in S/O atmospheres at 1000 to 1300°C with partial pressure of sulfur of the order of $\sim 10^{-6}$ bar and $p(O_2) \sim 10^{-15}$ to 10^{-20} bar. The weight changes with time have been measured, and x-ray diffraction studies show the β -Si₃N₄ and Y-N-apatite phases to decrease markedly with the formation of a noncrystalline SiO₂ (see van der Biest et al., 1987).

Mechanical Properties. Flexural tests of Si₃N₄-based ceramics are carried out by four-point bending techniques, modified to use cylindrical bearings with a constant stress distribution between the inner loading points. These tests can be carried out in air, vacuum, or controlled corrosive environments at temperatures up to 1500°C. Tensile tests are carried out using a gripping system consisting of a BN powder cushion around the head of the specimen to distribute the constant stress on the ceramic specimen.

Si₃N₄ densified with Y₂O₃ gives rise to a material with good retention of properties with values of strength of 600 MPa at 1400°C. The microstructure, as determined by transmission electron microscopy, shows the presence of a YSi₂N₂O phase, and an apatite structure at the grain boundary and at the triple points between the Si₃N₄ grains. These phases are completely crystalline after high-temperature treatment. In deformed specimens, a glassy phase is observed at the grain boundary. Long-term oxidation tests on Y₂O₃ hot pressed Si₃N₄ have been carried out, when there is an appreciable decrease in strength. The creep rate in N₂ is higher than in oxidizing environments. These results indicate that the creep resistance is improved by the removal of impurity elements by diffusing into the oxide layer.

Other Studies. Other studies at JCR Petten include:

- Ceramics for high-temperature heat exchangers (see Van der Biest et al., 1985).

- Ceramic coatings (see Van der Voorde et al., 1987).
- Corrosion resistant materials for coal conversion systems (see Norton et al., 1985).

Discussion

The corrosion studies at JCR Petten are part of a well-thought-out, coordinated program of the behavior of materials of industrial importance in realistic situations. There is a very good cooperation between university, research institute, and industry, extending across the national boundaries of Europe. The laboratory at JRC Petten is set up very carefully and very deliberately to be able to study the behavior of material under severe environments, and these studies should lead to a better understanding of the mechanism of the corrosion of materials.

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1/11/88

REFRATORIES MEETING IN GERMANY

Louis Cartz

Introduction

Refractories in the Chemical Industry and in Waste Incineration was the theme of the 30th International Colloquium on Refractories, held on 8 and 9 October 1987 in Aachen, West Germany. It was organized by Das In-

stitut für Gesteinshüttenkunde der Rheinische-Westfalen, Technischen Hochschule (RWTH) Aachen, das Forschungsinstitut der Feuerfest-Industrie, Bonn, and die Deutsche Gesellschaft für Chemisches Apparatewesen, Frankfurt/Mein. Of the more than 350 participants, most came from Germany, though some 120

came from some 20 other countries, including 25 from France, 17 from the UK, 16 from the Netherlands, and 12 from Belgium. Simultaneous translations in English, French, and German were available.

The meeting was held in the Kármán Auditorium of the RWTH Aachen. An ingenious large wrap-around projector screen enabled the simultaneous projection of several slides. The organizers of the meeting are to be complimented on overcoming the language barrier by the fine simultaneous translations, and for the complete proceedings published in advance.

The meeting, concerned with protective linings for furnaces, incinerators, pipes, and conduits, encompassed 17 talks, most of which lasted 30 minutes, and no posters. Most of the talks were concerned with practical systems, describing problems in the use of a range of furnaces, incinerators, and pipe systems. This limited the technical interest of the meeting. Little work was reported on microstructural features of the refractory linings.

The papers concerning refractory linings were of the most interest; therefore, this note will concentrate on them.

Refractory Linings

W. Krönert (Institut Gesteinshüttenkunde, Aachen, West Germany) discussed the stability of refractory linings containing Al_2O_3 and mullite used in furnaces for the chemical and petrochemical industries and for waste incinerators. Temperatures of 1000-1300°C are frequently attained, and the atmospheres can be highly reducing with the presence of alkali ions and also of V, Cr, S, and Zr. Krönert described the changes of eutectic temperatures which can decrease appreciably in the presence of impurities, resulting in complex phase systems. New phases such as $(\text{Na,K})\text{AlSiO}_4$ (nepheline), $\text{Na}_8\text{Al}_6(\text{SiO}_4)_6(\text{SO}_4)$ (nosean), $\text{Na}_4\text{Al}_3(\text{SiO}_4)_3\text{Cl}$ (sodalite), and $(\text{Na,Ca})_{4-8}(\text{Al}_6\text{Si}_6)\text{O}_{24}(\text{SO}_4)_1.2$ (hauyne) can form. These precipitate in the pores of the lining, resulting in changes in thermal expansion and thermal shock characteristics.

Very little data were described on the testing of materials outside their actual use in incinerators or furnaces. Some data were reported by E. Ruhl (Lurgi Chemie und Hüttenwerke GmbH, Frankfurt, Germany) on crucibles materials from tests of their stability at temperature to certain fuels and wastes, but these tests were only of a rudimentary nature. He also reported some work on mockups of small furnaces.

R. Krebs (Linco-GmbH, St. Augustin-Hangelar, Germany) described three examples of problems arising in the use of refractory linings where the operating temperatures can be higher than expected, slag softening occurring at lower than expected temperatures, and attack by corrosive gases can occur. The first example was

that of a protective coating (95 percent Al_2O_3) for pipes used for gases. These linings developed hotspots leading to breakdown due to chloride formation. This was diagnosed as coming from the water used in the preparation of the corundum concrete binding the protective coatings. The second example was that of a waste incinerator for chipboard dust and wood waste products. The slag composition was very far from what had been anticipated and had a flowpoint, determined by hot-stage microscopy, of 1350°C—much higher than the 1100°C expected. The third example was in the incineration of liquid wastes from the residues of molasses, giving rise to ethane. The residue from sugar cane gives rise to ' SO_4 ' and CaO , whereas the residue from sugar beet gives rise to ' SO_4 ' and K_2O . The furnace design for sugar cane residue was found not to be serviceable for sugar beet residue for this reason. Krebs pointed out that there was an enormous amount of ash produced by sugar beets so that the furnace required frequent cleaning. This led to mechanical damage and to increase in thermal shock, resulting in early damage to the lining.

There were a few papers that discussed new materials. J. P. Moreau (Lafarge Refractaire Monolithique, Montrouge, France), described the development of linings based on concrete containing much smaller amounts of cement binding materials: low cement castables (LCC) and ultralow cement castables (ULCC). Normal concrete uses 20- to 30-weight percent of cement and consequently contains 5- to 10-weight-percent CaO . The ULCC uses 1- to 2-weight-percent cement and consequently 0.5- to 1-weight-percent CaO . Trials of the LCC and ULCC linings are continuing.

Discussion

Most participants used the meeting to make personal contacts with others members of the refractory lining industry. There was certainly the opportunity to hear of typical problems with the refractory linings and some solutions. However, the scientific content and technical development were not prominent at this meeting. Virtually no papers were presented from universities or research institutes. Almost all of the papers were from industries, and concerned actual industrial situations.

Many speakers described extensive chemical examinations of the refractory linings being used, which were mainly alumina- or mullite-containing ceramics. Many of the problems in working systems were diagnosed as due to:

- Incorrect temperature measurements
- Thermal shock due to the necessity of frequent cooling to cope with situations such as the removal of ash
- Excessive damage to the refractory linings due to liquid slags running constantly over the lining surfaces
- Mechanical damage during the removal of slags

- Variable and unexpected chemical compositions of the waste being incinerated
- Thermal shock when liquid wastes are sprayed into the furnaces.

Two points of interest were the following:

- Temperature measurements at 1300-1500°C present difficulties in practical situations, and frequently the measurements do not correspond to reality since the linings have obviously melted.

- Modeling of furnace lining situations was discounted as not being satisfactorily performed. However, such modeling, if properly carried out, would be most helpful.

12/24/87

PHYSICS

Quantum Optics, Optoelectronics, and Laser Spectroscopy at the General Meeting of the European Physical Society

by Paul Roman. Dr. Roman is the Liaison Scientist for Physics in Europe and the Middle East for the Office of Naval Research's London Branch Office. He is on assignment until September 1988.

The European Physical Society (EPS)—a loose association formed almost 20 years ago of European national physical societies and some other professional groups—held its Seventh General Conference (EPS-7) from 10 through 14 August 1987 in Helsinki, Finland. While the official sponsor was, of course, the EPS, most of the fiscal burden was carried by the Finnish Physical Society and a number of Finnish educational, cultural, and private business groups. The host institution was the Helsinki University of Technology; its modern, spacious campus in Otaniemi, Helsinki's new western suburb, provided a fine background, and commuting to Helsinki proper was not too cumbersome. There were around 800 participants, including, naturally, a higher proportion of Soviet and Iron-Curtain country scientists than is customary at single-topic European conferences. Special efforts were made to ensure the participation of an unusually high contingent of very junior colleagues. There was a small, well-setup exhibition by firms that supply research equipment to universities (Finnish firms dominated); the most interesting exhibit was a joint show by Finnish firms and the Helsinki University of Technology, illustrating participation in the European high-energy accelerator project LEP at the European high-energy research center (CERN) at Geneva. Guided lab tours to selected research units of Helsinki University of Technology added further highlights and improved person-to-person exchanges.

The programing had an interesting structure. In the mornings (and all day on the last day) 45-minute-long plenary session talks by distinguished speakers reviewed

the current status of a discipline or summarized current research in a rapidly developing field. The subjects of these representative presentations ranged from superstring theory and optical computers through submillimeter wave spectroscopy and polymers to Halley's Comet and point-contact spectroscopy of metals. (Somewhat incongruously, there was also included a presentation by N. Blombergen [Harvard University, Cambridge, Massachusetts] who recounted the essence of the American Physical Society's recent study on the role of laser and particle beam weapons in the SDI program). Altogether, there were 21 plenary talks.

After the lunch breaks, well-focused symposia took place. Unfortunately, there were always five of them (once even six) running in parallel. Each symposium had one or more invited talks (30-45 minutes long) and several contributed papers (15 minutes each, but some of them displayed only in special poster sessions). In addition, there was an alarmingly large number of unrelated posters on "general topics," displayed in late afternoon timeslots. Finally, most evenings there were reports and discussions on topics of particular EPS concerns.

I find it useful to list the titles of the 17 Symposia, because this list reflects well the breadth of the physics research in Europe:

- High energy and particle physics
- Laser spectroscopy
- Hot carriers in electronic devices
- Physicists [sic] in brain research
- Cyclotron resonance of electrons in two dimensions
- Plasma treatment of surfaces: science and technology
- High-temperature superconductivity

- New aspects of nuclear structure
- Dynamics of excited atoms and molecules in collision
- Quantum optics: two-dimensional structures and single particle systems
- Heavy fermions
- Physics of ultrashort optical pulses
- Physics and modern production technologies
- Modern computations of molecular structure
- Scanning tunnelling microscopy
- Physics and Society
- Physics in developing countries.

In this article I review only briefly some representative talks in the area of quantum optics, optoelectronics, and laser spectroscopy.

Progress in Quantum Optics and Electro-Optics

For me, the most exciting talks on these subjects were in the area of single-atom masers—i.e., the quantum electrodynamics of a single atom in a cavity, where it interacts with a single mode of a resonant electromagnetic field. As is well known—and as well publicized at several conferences in the last 3 years—pioneering work in this area was done at the Max Planck Institute for Quantum Optics at Garching (West Germany), under the inspiring leadership of H. Walther. In his talk at Helsinki, Walther emphasized strongly that, since the atoms in the experiments are in very high Rydberg states and are enclosed in a superconducting cavity, the relaxation time of the cavity field is larger than the characteristic time of the atom-field interaction (the latter being given by the reciprocal of the Rabi frequency). He then explained how the statistical and discrete nature of the photon field leads to new dynamic characteristics. In particular, Walther discussed recent results regarding the collapses and revivals in the Rabi nutation.

Closely connected to this talk was the presentation by M. Brune on behalf of the Ecole Normale Supérieure (Paris, France). Brune pointed out that the Rydberg atom-field coupling in the cavity may be so strong that the system can even oscillate on nonlinear two-photon transitions, in a regime where each atom emits a pair of photons in the cavity. This is important, since continuous two-photon amplifiers with large numbers of atoms and photons could not be realized until now. Brune quoted recent theoretical calculations that indicate a number of interesting quantum properties which would show up in a microscopic two-photon Rydberg maser. For example, the phase diffusion of the field and its fluctuations will be quite different from those in a one-photon maser. Finally, Brune described progress at his institute in actually building a two-photon micromaser which uses Rb atoms as the active medium and a Nb superconducting resonator as the maser cavity.

In another, currently exciting area, D. Paquet (CNET, Bagnex, France) gave an interesting theoretical discussion of both known and expected optical properties of semiconductor superlattices. He showed how the striking features of the electronic structure can be derived from tunnelling between states confined within quantum wells. The electronic structure, in turn, drastically influences optical properties. Paquet paid special attention to excitonic properties and the role of impurities, interface roughness, and strained layers. While, as far as I can see, the talk did not reveal surprises, it gave a very clear, general view of, and approach to phenomena usually not treated in a uniform framework.

R.M. Nieminen (Helsinki University of Technology, Finland) also talked on electronic properties of two-dimensional systems. This was a good theoretical study of peculiar quantum consequences of lowered dimensionality in such phenomena as the quantized Hall effect. Applications to device physics were very clearly elucidated.

Two presentations from the Nonlinear Optics Division of the Poznan University's Institute of Physics (Poland) were concerned with squeezed states and photon antibunching. The first, by Z. Ficek and S. Kielich reported on anomalous coherence functions in transient resonance fluorescence. The second, by M. Kozierowski, discussed the anticorrelation effect and showed how in second-harmonic generation this leads to the violation of the Cauchy-Schwartz inequality predicted by classical theory. Personally, I do not think that these contributions contained genuinely new or interesting material.

However, a third presentation from the same Polish research center (signed by Z. Ficek, P. Chmela, and S. Kielich) deserves commendation. These scientists reported on enhanced incoherent sum-frequency generation (SFG) by group-velocity difference. Actually, they proposed a theoretical model of optical SFG by incoherent nonlinear mixing of two beams, one being coherent and the other chaotic with arbitrary intensity and spectral width. The efficiency of SFG was calculated in the second approximation of an interactive method which solves the equations of parametric interaction of the three waves. The result was analyzed in terms of a number of experimentally controllable parameters.

Ultrashort Pulses

There was a wealth of talks in this area and I select, somewhat randomly, only those which addressed fundamental issues and appealed to me particularly.

J.R. Taylor (Imperial College, London, UK) talked about femtosecond pulse generation through soliton-Raman processes. On behalf of several scientists in the Laser Optics Group, Taylor reported on the generation of tunable, high-power femtosecond pulses using the par-

ticular soliton-Raman pulse formation mechanism first proposed by Soviet authors. Several experimental schemes were described in the talk; the experiments all used 100-ps pulses from a CW mode-locked Nd:YAG laser operating at $1.32\text{ }\mu\text{m}$ as the pump source. Single-pass operation as well as soliton relaunch and reconstruction through synchronous amplification were considered in the report. In addition, Taylor described simple soliton-Raman fiber ring oscillators and also a cascade Raman soliton system which permits tunable operation from $1.32\text{ }\mu\text{m}$ to $1.7\text{ }\mu\text{m}$ with 100-fs pulses in the kilowatt power range.

The talk given by H.P. Weber (University of Berne, Switzerland) attacked a related problem. He reported on the propagation of subpicosecond pulses and soliton formation in an optical fiber. While the parts of the talk concerning spectral broadening and frequency chirping of pulses, on undisturbed propagation of optical solitons, and on the soliton self-frequency-shift contained little novelty, the detailed theoretical and experimental analysis of the disintegration of pulses into a set of fragments with soliton nature covered many new results.

The next two talks I review were more in the area of applications.

G.M. Gale (Ecole Polytechnique, Palaiseau, France) talked about the dynamics of picosecond phonon-polariton pulses. He recounted that his group's work on coherent optical picosecond pump- and probe-techniques has been recently extended to the investigation of the dynamics of phonon-polaritons in crystals. These nonlocal experiments, Gale told us, not only allow the study of polariton time-decays due to interaction with bulk-crystal modes, but also give access to the spatial propagation of picosecond pulses of these elementary excitations inside the crystal. Consequently, one may observe the scattering of polaritons from spatial inhomogeneities, and one can study their behavior at and beyond the crystal surface.

The talk by V. Brückner (University of Jena, East Germany) took us out of the realm of pure optics, since it considered the exciting possibilities of picosecond optoelectronic semiconductor switching. Brückner described new experimental and theoretical studies in the area of ultrafast optoelectronic switches, such as: linear and nonlinear recombination, carrier mobility and drift, and multistep and multiphoton absorption; circular electrodes, finger structures, and inhomogeneous optical and electric field distributions; and backside and inhomogeneous illumination. He also described some new methods for the generation of picosecond electric pulses by the use of picosecond lasers, such as the use of semiconductors with fast recombination time (amorphous GeSi and Si, doped H:a-Si, GaAs, GaSe). Attention was paid to the method of what he called partly covered gap and inhomogeneous gap excitation methods in semicon-

ductor superlattices. Several practical applications concluded the impressive report. These included the following areas: studies of transport processes in amorphous and monocrystalline semiconductors; generation of ultrashort electrical pulses with kilovolt amplitudes; measurement of pulse dispersion in cables; and response time measurement in active and passive electronic elements (such as diodes and transistors) in the GHz range. The depth and breadth of Brückner's talk indicates, I think, the seriousness of fast-electronics research at Jena.

Laser Spectroscopy

There were only two oral presentations in this area (and a somewhat unfocused roundtable discussion); the majority of contributions were presented in a poster session. I pick only a few samples.

W. Demtröder (University of Kaiserslautern, West Germany) reviewed recent progress in laser spectroscopy of molecules. Demtröder emphasized that the combination of high-resolution laser spectroscopy with molecular beam techniques and adiabatic cooling of molecules during the supersonic expansion has brought about considerable achievements in simplification of complex molecular spectra and their analysis, even for very large molecules. (Example: production and spectroscopy of metal clusters in cold noble gas supersonic beams seeded with metal vapor.) Another interesting field in the area concerns the study of molecular Rydberg levels and their interactions. (Example: recent experiments on diatomic alkaline molecules.) Finally, attention was called to new possibilities for time-resolved spectroscopy of fast relaxation processes. (Examples: lifetime measurements under collision-free conditions, studies of intermolecular energy transfer, collision-induced relaxation.) The well-organized talk was mostly tutorial and I found it difficult to discern which results referred to work specifically done at Kaiserslautern.

One of the topics noted in Demtröder's review was well illustrated by a presentation from the University of Bayreuth (West Germany), submitted by A. Laubereau, H. Graener, and R. Dohlus. This work concerned itself with time-resolved infrared double resonance spectroscopy of liquids, using tunable ultrashort (picosecond) light pulses and weak probing pulses. Apparently, this was the first successful attempt at obtaining ultrafast probing spectra in the infrared. Examples were presented on results with CHBr_3 and on $\text{C}_2\text{H}_5\text{OH}$ in solution of CCl_4 . Direct evidence was obtained for the picosecond-time-scale breaking of hydrogen bonds after infrared excitation; and also evidence for energy transfer from OH to CH stretching modes.

J. Pantoflíček, M. Urbanová, and P. Klíma (Charles University, Prague, Czechoslovakia) submitted a report that describes an interesting infrared study of color

centers in LiF crystals. The γ -irradiated samples' infrared absorption spectra in the 1500-3200 cm^{-1} range showed (not unexpectedly) changes depending on the density of the color centers. The absorption of the OH-groups and the role of oxygen in the color center formation were studied in some detail.

Another contribution to the area of applications was submitted from the Chalmers University of Technology, Göteborg, Sweden, by a larger group of scientists, under the lead of S. Ljungström. The scientists used laser-induced fluorescence techniques for the detection of intermediate OH radicals in the oxidation of hydrogen to water on a polycrystalline Pt foil. (The production of water was simultaneously measured by evaluation of the chemical energy released at the catalyst.) The most interesting result of the study was that the H-burning does not proceed according to the most commonly assumed schemes, but rather via the $\text{OH} + \text{H} \rightarrow \text{H}_2\text{O}$ process taking place on the Pt surface.

Concluding Comments

The EPS-7 conference (subtitled, quite correctly, "Trends in Physics") was a success. It brought together

many experts and young scientists from a large number of fields. The plenary talks were of exceptionally high quality. Time-keeping was good and activities were neither hectic nor crowded (except perhaps the breaks and social gatherings). The atmosphere was friendly and cooperative – not automatically guaranteed at an all-European meeting.

I have the complete program (including poster titles) and almost all abstracts of talks and poster presentations. I also have a good, small booklet describing the exhibitors' firms. I will be glad to supply xerographic copies of well defined areas to interested colleagues.

The proceedings of the conference will be published in a special issue of *Physica Scripta* (journal of the Royal Swedish Academy of Sciences, P.O. Box 50005, S-10405 Stockholm, Sweden). Scheduled for the first quarter of 1988, it will contain the full texts of only the plenary and the invited talks.

8/25/87

Advanced X-ray Research at Garching

Paul Roman

Europe's leading quantum optics and laser research facility is the Max Planck Institute for Quantum-Optics, located at Garching (near Munich) in West Germany. In 1985 and 1986 I reported on the general and basic research groups and projects (see *ESN* 39-4:165 [1985] and *ESN* 40-9:287-290 [1986]). In this article I will review the work of a somewhat more specific research group, which is under the direct supervision of Dr. R. Sigel. This group, comprising about 10 members (including short-term visitors from both Japan and Eastern Europe), is primarily interested in the creation, detailed study, and possible use of soft x-rays produced by laser techniques. Related research in other areas is also pursued. While these endeavors do not lie in the areas which I habitually monitor, I find it well-advised to give a survey of them because, in my (perhaps not expert) opinion, this is truly outstanding research, done with the traditional patience, care, and in-depth exploration characteristic of continental European scientists.

Laser-Generated Intense Black-Body Radiation

I start with reporting on the most unconventional topic pursued by Sigel and coworkers.

General Background. Until recently, it has not been possible to generate Planck radiation in the laboratories with temperatures exceeding 10^4 or 10^5 K. The reason for this was that, according to the Stefan-Boltzman law, for a temperature of 10^6 K an enormous radiant energy flux of 6×10^{12} W/cm^2 is predicted, and the losses which arise when such high fluxes of radiation circulate are so high that the radiation field cannot be maintained by ordinary power sources. However, recent advances in pulsed lasers (and particle beam sources) offer the possibility for solving the problem and generating in a cavity Planck black-body radiation corresponding to 5×10^6 K. Possible specific applications of such Planck radiation are: the generation of an intense soft x-ray source, the laboratory study of radiation hydrodynamics, and experiments in a new range of high pressures; these topics are, of course,

closely related to energy production by thermonuclear fusion.

The basic method used at Sigel's lab (and at the labs of collaborating Japanese groups) consists in delivering a laser pulse into a mm-size cavity enclosed by a solid wall. One or more small holes in the wall are required for transmitting the beam. The rapid deposition of energy in the cavity will heat the inner wall to a high temperature and generate intense Planck radiation in equilibrium with the wall. It is necessary to ensure that the radiative exchange of energy between wall elements be so effective as to establish very uniform conditions in the cavity, even if the initial wall irradiation by the source is not uniform. Furthermore, the radiation field should be formed in the empty cavity before it fills with evaporated, hot plasma from the wall.

Theoretical Studies. Crucial for the success of the scheme is, of course, the confinement of the radiation by the cavity. Here a theoretical problem arises: there do not exist materials which would reflect effectively the soft x-rays (that dominate the Planck distribution at the considered temperatures). The incident photon-flux is completely absorbed by the inner surface of the cavity wall. Equilibrium can exist only between the radiation field and this hot layer or the inner surface of the wall which re-emits the absorbed incident energy. Thus, a fraction of the available energy is always used for reheating the wall material.

The complicated nonstationary hydrodynamic equations (including radiative heat transfer) that govern the situation had to be solved and carefully analyzed before the difficult experiments were to begin. Indeed, the first results have been reported in a paper by Sigel and R. Pakula (*Zeitschr. f. Naturforschung*, 41a [1986], 463-467). In this work, the credible assumption was made that local thermodynamic equilibrium (LTE) exists between radiation and matter. The LTE assumption reduces the mathematical difficulties to such an extent that the scaling laws for the temperature can be obtained immediately by dimensional analysis from the governing parameters of the problem. In order to obtain numerical results which would apply to the actual experiments, it was assumed that the cavity wall is a high-Z material (such as gold). It would lead me into much too specific details if I were to report the entire analysis. Suffice to say that the authors became convinced that, with a 10^{-7} to 10^{-9} -sec-long laser pulse, containing 10^{12} -erg energy, a temperature of about 5×10^6 K may be surely achieved. In this estimate, the cavity was taken to have a 2-mm radius. It was also calculated that with an irradiation at 10^{14} W/cm², heating will self-terminate after about 2 ns. By then about 30 re-emissions would occur, and the total laser energy delivered into the cavity would total 10^5 J.

Experimental Results. These careful theoretical studies were followed by exiting experiments. The laser source was the world's leading iodine vapor laser at Garching (operating at 1.3 μ m). Spherical gold cavities with 0.25 to 1 mm diameter were irradiated with 0.3-ns pulses. The cavities had one hole for admitting the laser beam, and one, smaller, diagnostic hole; the radiant energy flux and the spectrum of the cavity radiation was measured. Temporal resolution was achieved by a specifically developed soft x-ray camera. One result was that for the lowest flux used (2×10^{12} W/cm²) the x-ray emission occurs preferentially around 50 Å; for the highest flux (3×10^{13} W/cm²) the peak is at 20 Å. This shift is not unexpected: it corresponds to the shift in the emission of a Planck radiator with increasing temperature. For an absorbed laser energy of 20 J, a radiant energy flux in the cavity corresponding to a brightness-temperature of 1.3×10^6 K was observed. While these and other observations agreed well with the calculations, the intensity of the radiant energy flux of the cavity was less by a factor of 0.8 to 0.3 than the predicted flux. Obviously, the laser falls short of the ideal source assumed in the calculations: part of the energy is lost into nonradiative channels.

A preliminary report on these fine experiments has been published by the research group in *Europhysics News* 17 (1986), 116-120. Additional details maybe found in *Europhysics Letters*, 2, (1986), 213-219. A more specific analysis, focusing on the temperature measurements of the laser-heated cavities and their comparison with theoretical work, was published in the *Zeitschr. f. Naturforschung*, 41a (1986), 767-768. An interesting aside to the main research was a shadowgraphy study of the outward motion of the thin wall of the laser-heated gold cavity. A six-frame optical and a single-frame x-ray back-lighting technique was used, and it was concluded that the measured velocities can be attributed to the pressure produced by an ablative heat-wave which is driven into the wall by thermal soft x-ray radiation generated in the cavity. (This investigation was reported in *Europhysics Letters* 2, [1986], 221-226.)

Soon after the Garching experiments were well underway, the Sigel group also joined colleagues engaged in similar research at Osaka University (Japan). The research was actually conducted at the Institute for Laser Engineering. Here a frequency doubled Nd: Glass laser (Gekko XII) source was used, providing more energetic laser pulses; and also, larger cavities (0.6- to 2-mm diameter) were used. The laser pulses (at 0.53- μ m wavelength) had 300-ps duration and delivered 3-kJ energy. The major result of these (still ongoing) experiments was that a higher brightness temperature, 2.2×10^6 K, has been obtained. A short preliminary report can be found in the *Proceedings of the 11th International Conference on Plasma Physics and Controlled Nuclear Fusion Research*,

International Atomic Energy Agency Report CN-47/B-I-3, (1987).

X-ray Spectral Measurements

Another noteworthy line of research in Sigel's group, more on traditional grounds, is the spectrum analysis of soft x-rays emitted by laser plasmas.

A group of seven researchers (including Sigel, Pakula, and one of the Garching Directors, S. Witkowski, as well as a Japanese visitor and a researcher with the Siemens Laboratories) recently developed a technique for absolute measurements of the 50-eV to 1000-eV soft x-ray emission from laser plasmas. The experiment was done by using transmission gratings, including pinhole-grating combinations for spatially resolved spectroscopy. The film was absolutely calibrated with the help of a bolometer, the laser plasma itself being used as a source.

In a related work, K. Eidmann and T. Kishimoto made absolute measurements on the soft x-ray spectra emitted by laser-produced plasmas in the wavelength range 10 Å to 250 Å. Here also a transmission grating and

a calibrated film was used, but the scope of the study and the technique was more sophisticated. The 0.53-μm laser pulses with a 3-ns length (obtained from a frequency-doubled Nd:YAG laser) were focused at an intensity of 3×10^{13} W/cm² on planar targets of various elements with Z ranging from 4 to 82. The major result was that the overall conversion of incident laser energy into x-ray energy increased from 2 percent (for Be) to as high as 50 percent (for many of the heavier elements).

Concluding Remarks

While I was very brief on describing activities outside the Planck radiation studies, this in no way implies a lack of dedicated work relating to various aspects of x-ray emitting plasmas. In any case, I feel that the Sigel group is in the frontline of advanced European research with x-ray generation by very modern techniques, and deserves much credit.

2/14/88

12TH INTERNATIONAL CONFERENCE ON AMORPHOUS AND LIQUID SEMICONDUCTORS

by P. Craig Taylor and James A. Freitas, Jr. Dr. Taylor is a Professor of Physics at the University of Utah and Dr. Freitas is in the Electronics Science and Technology Division, Naval Research Laboratory, Washington, DC.

The 12th International Conference on Amorphous and Liquid Semiconductors was held at the Palace of Culture in Prague, Czechoslovakia, from 24 through 28 August 1987. The first in this series of conferences, also held in Prague, took place in 1965, and successive conferences have been held every 2 years since. While the first conference drew about 50 participants, this last one was attended by over 800. Approximately 350 papers were presented, either orally or in poster sessions, during the 5 days of the conference.

As has been the case in recent conferences in this series, the vast majority of the papers concerned hydrogenated amorphous silicon, a-Si:H and related tetrahedrally-coordinated amorphous alloys. Semiconductor glasses, such as the chalcogenide glasses, and liquid semiconductors represented only about 10 percent of the program. The great, and perhaps disproportionate, interest in a-Si:H is of course due to the usefulness of this material in devices such as large-area solar cells, thin film transistors, photoreceptors, and so forth.

The major topics discussed at the conference were:

- Transport properties, including the nature of the mobility edge, localization theory, and band tail states

- Structure, including order beyond the nearest neighbors
- Defects and electronic states deep in the gap
- Optical properties and photo-induced phenomena such as the Staebler-Wronski effect in a-Si:H and photodarkening in the chalcogenide glasses
- Materials properties such as sample preparation, especially in tetrahedrally coordinated alloys based on a-Si:H
- Interfaces
- Multilayers and heterostructures, especially in tetrahedrally coordinated alloys
- Devices based on a-Si:H and related alloys.

Among the controversial ideas most hotly debated at the conference were the possible occurrence at low temperatures of mobilities $> 1 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ in a-Si:H and the attribution of the dominant paramagnetic defect on a-Si:H to an unpaired electron or a five-fold coordinated silicon as opposed to a three-fold coordinated silicon. Also debated were the fundamental mechanisms causing hydrogen diffusion in a-Si:H, and the microscopic mechanism for photodarkening in the chalcogenide glasses.

Professor Spear and his colleagues (University of Dundee, UK) reported transport measurements of films of a-Si:H which were interpreted in terms of a rise in the mobility of the carriers to values greater than $1 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ at temperature below 100 K. The question of how this value for the mobility can be reconciled with the hopping transport mechanism long thought to dominate at these low temperatures in an obvious one. Professor Mott (University of Cambridge, UK) discussed some recent developments concerning the nature of the mobility edge in amorphous semiconductors, including the suggestion at the conference of Professor Thomas (University of Marburg, West Germany) that the current path is above the mobility edge.

Several sessions at the meeting were devoted to discussions of order in amorphous semiconductors beyond that determined solely by nearest neighbors. Order beyond nearest neighbor is sometimes called "medium range order." Even for specific amorphous semiconductors, this conference provided no coherent definition of what such medium-range order encompasses. Professor Lucovsky (North Carolina State University, Raleigh) did suggest a mechanism which might drive medium-range order in the chalcogenide glasses, namely the relative orientation of the lone-pair chalcogen orbitals.

Perhaps the most controversial suggestion of the meeting came from Dr. Pantelides (IBM, Yorktown Heights, New York), who proposed that the dominant paramagnetic defect deep in the gap in a-Si:H is an electron centered on a fivefold coordinated silicon atom, usually called a dangling bond. The "floating bond" provided the focal point for much intense, and sometimes

heated, discussion both in the sessions and in the hallways.

The general question of hydrogen diffusion in a-Si:H and the potential role which this diffusion might play in producing nonequilibrium configurations in a-Si:H were also an important focus of the meeting. Dr. Kakalios presented data from the group at the Xerox Palo Alto Research Center, California. He interpreted these data as implying that hydrogen diffusion can explain all of the observed nonequilibrium phenomena in a-Si:H. This interpretation also provided a focal point for some hearty dissension. A slightly different perspective was presented by Dr. Smith (Princeton University, New Jersey) who suggested that the freezing in of broken silicon-silicon bonds was of primary importance in explaining many nonequilibrium phenomena in a-Si:H.

In that small portion of the conference which did not involve the tetrahedrally coordinated amorphous semiconductors, the topics which received most interest were photodarkening and photodoping in the light-enhanced diffusion of metal atoms through many chalcogenide glasses. Several microscopic models for photodarkening were discussed at this conference, although there was no general agreement as to which model, if any, might ultimately prove to be correct.

As has been the case for the last few of these conferences, there was little time spent on liquid semiconductors. One session on the last afternoon covered this entire field.

3/2/88

TOPICAL SYMPOSIUM ON SYNERGETICS DRAWS 80 INTERNATIONAL SCIENTISTS TO MADRID

Paul Roman

A number of youngish, established Spanish scientists are vigorously campaigning to enhance the image of Spanish science in areas where it can really show off its fine achievements. One of the best known among these campaigners is Professor Manuel Garcia Velarde, a theoretical physicist, the head of the Basic Physics Department at the National Open University (Universidad Nacional de Educacion a Distancia [UNED]), located in Madrid. Velarde was drawn to general studies in nonlinear dynamics from his original, more specific interests in fluid dynamics. He not only built up connections with leading international experts on nonlinear dynamics, but now also has in his department a good work-group, engaged both in theoretical and experimental research in this burgeoning area. Velarde led a suc-

cessful fight for establishing a new science laboratory center, serving all of UNED; and, after some delays, this research center was completed in the fall of 1987. Velarde then capitalized on this achievement by organizing an international meeting for the occasion of the inauguration of the center. The "International Symposium on Synergetics, Order, and Chaos in the Natural Sciences, Mathematics, and Other Sciences" took place in Madrid from 13 through 17 October. It was cosponsored by UNED and the Fundación Ramón Areces, a private research-support foundation. The Ministry of Education and Research, as well as a few private industrial firms, gave additional logistical support.

While this was a "by invitation only" meeting, there were over 80 participants. The number proved ideal for

a topical conference, and in fact, during the sessions that took part not in the new fine Aula of UNED but in the downtown convention room of the Fundación, there was even some crowding. More than one third of the participants came from various Spanish universities, showing the popularity of synergetics in Spain. The other participants came from all leading Western European countries; there were also three Americans. The Peoples Republic of China was well represented, as well as Hungary. But the two invited Soviet speakers sent a last-minute telegram, stating that they did not get the necessary exit permit from their Academy of Sciences. (So much for Glasnost.)

There was an amazing number of lectures: 40 in all. It was possible to accommodate these talks, without exhausting the audience and without splitting up into parallel sessions, by utilizing the peculiar Spanish working-hour system: a late 9:30 a.m. start, a substantial midday break, and reconvention at 4:30 p.m., with the session then going on until about 9:00 p.m.

The inauguration session commenced with the keynote-address by H. Haken (Stuttgart University, West Germany). Actually, Haken (well known as the "inventor" of the synergetics concept and its most vigorous apostle) was a special guest of honor and, during a most festive university convocation, was presented with an Honorary Doctorate by UNED.

Haken's talk (taking a leisurely hour's span) first illustrated the concept of self-organization in systems varying from galaxies through liquids to living organisms, large and microscopic. Then he turned to the more mathematical part of his presentation, explaining past research aimed at the unveiling of general laws that govern self-organization. In the last part of his talk Haken described his current work, which is based on the thesis that pattern recognition is reciprocal to pattern forming and therefore may be attacked by methodology developed in the area of synergetics.

The other two talks in the inaugural session (lasting 45 minutes each) were given by D. Avnir (Hebrew University, Jerusalem, Israel) and A. Mandell (University of California, San Diego). Avnir described how chemical reactions may induce hydrodynamic instabilities. In turn, Mandell covered a biological terrain: his talk carried the exciting title "The Evolutionary Selective Genetic Apparatus as a Dynamical System."

The other 37 talks (each of 30 minutes) ranged over a bewildering area. We heard reports ranging from rather standard topics such as "anomalous diffusion and chaos," "cellular solidification as a bifurcation problem," or "turbulent hydrodynamic oscillators" to "chaotic dynamics of biological information processing" and "phase transformations with cellular automata." Actually, the talks were not (possibly could not easily have been) organized into transparent sequences, and it is not profitable to randomly select some for analysis.

As a matter of fact, this was an "insiders" conference. There were not even nametags issued, because the assumption was that everybody knows everybody. (Not quite so!) While good mixing of people was possible during the long breaks, the sessions were often hectic; the scheduled times were not taken seriously and the entire preparation and organization of the symposium showed some signs of chaos (pun intended.) But the well-known Spanish pleasantness smoothed out rough corners.

The scientific level and seriousness of the presentations varied significantly. On the whole, it seems that the in-depth study of nonlinear phenomena reached a degree of maturity.

There were no abstracts issued, but the full talks will be collected in a forthcoming special volume of the well-known Springer-series, *Synergetics* (editor: H. Haken).

I have a list of participants (with full addresses) which I would gladly share with interested colleagues.

10/20/87

CORRELATION, ORIENTATION, AND SPIN EFFECTS IN ELECTRONIC AND ATOMIC COLLISIONS – AN ONRL-SPONSORED WORKSHOP

Paul Roman

Research on polarization and correlation in atomic collision physics has an impressive history that started by studying electron-electron coincidences, electron-photon coincidences, and electron-spin effects. Impact processes with ions and atoms as projectiles, and electron collisions with molecules, followed soon. More recently, approaches to "complete experiments" have been

reported in photoionization of atoms by applying spin-polarized atoms and electron spin analysis of photoelectrons. Further along the line, alignment, orientation, and electron-spin effects have even been studied in chemical reactions with aligned molecules. Many other developments are in the making in the area of future research projects aimed at extracting maximum informa-

tion on the collision process, gleaned by the analysis of polarization and correlation of atomic collision processes.

The current enthusiasm of researchers in this field was the motivation for organizing at the Queen's University of Belfast, Northern Ireland, UK, an International Symposium in Electronic and Atomic Collision. This symposium was held on 30 and 31 July 1987, immediately following the International Conference on the Physics of Electronic and Atomic Collisions, at Brighton, England, so that it was essentially a satellite meeting. The directors of the Belfast symposium were A. Crowe and M.R.H. Rudge, both from Queen's University. There were over 50 participants. On the second day, a special Workshop on Correlation, Orientation, and Spin Effects was held; this session was supported in full by the London Branch Office of ONR. The four invited talks lasted 45 to 60 minutes each. Following is a brief review of those four presentations.

N. Andersen (University of Aarhus, Denmark) talked about propensity rules for orientation in heavy-particle collisions. The presentation concentrated on recent progress in the understanding of the physical origin of the orientation of atomic states for direct excitation by heavy-particle impact. Andersen showed that theoretical analysis of the simple model-case of SP excitation leads to the formulation of a propensity rule for the orientation, valid at the impact velocity where excitation is most important. He pointed out that experimental results support the theoretical predictions and illustrate the validity range of the propensity rule. Finally, various generalizations and their experimental implications were discussed.

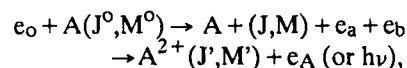
In a presentation entitled "Angular Momentum Coupling in Atom-Atom Collisions," J. Grosser (Hannover University, West Germany) discussed the coupling between the electronic wave function and the rotating atom-atom axis in an atom-atom collision. Both the orbital and the spin degrees of freedom of the electrons were considered. Grosser described the collision process as a sequence of simple angular momentum coupling problems so arranged that the transitions occur at localized transition regions. Analytical results, which can be compared directly with the results of appropriate experiments, were derived for various types of transitions.

E. Reichert (University of Mainz, West Germany) talked about experiments by investigators in Mainz with polarized electrons. He had two distinct areas to cover. The first concerned (ns-np) excitations of alkali atoms by polarized electrons where some of the spin orientation of the primary electron beam is transferred to the atoms because of exchange collisions. In particular, the scientists studied the polarization transfer to K, Rb, and Cs, respectively, by looking for the circular light polarization of (np-ns) decay radiation emitted in forward direction and

following impact of the atoms by a beam of longitudinally polarized electrons. Maximum polarization transfers were observed at collision energies that are about 1.5 times that of np-thresholds. The transfer increases with increasing atomic number. In the case of (6s-6p) excitation of cesium, 45 percent of primary electron spin polarization is transferred to the atoms at maximum polarization. The experimental data agree satisfactorily with available close-coupling calculations.

The second set of experiments reported by Reichert are more interesting to "high energy" theoretical physicists: these experiments considered parity violation in electron-nuclear scattering. It is now generally accepted that the electron interacts with an atomic nucleus not only via Coulomb forces but, in addition, via weak forces which are mediated by the neutral heavy Z^0 gauge-boson. The weak contribution to electron scattering is extremely small at atomic or even nuclear energies, but may be detected by taking advantage of the parity violation of weak forces. Reichert's work measured parity violation in electron-beryllium scattering at 300 MeV and at backward angles. The researchers were observing the dependence of the quasi-elastic cross section on the electron helicity. An "analysing power" of 1.6×10^{-5} was measured, which is in agreement with predictions of the so-called standard model of the electroweak interaction.

Postcollision interactions in ejected electron-pair and electron-Augur experiments were the topic of the concluding talk, presented by A. Lahmam-Bennani (University of Paris, Orsay, France). The reactions under investigation were of the type



where the indexes o, a, b, and A, respectively, stand for incident, (fast) scattered, (slow) ejected, and Auger electrons. Both outer- and inner-shell ionization processes were investigated. For outer shells, the scattered and ejected electron pair was observed in coincidence and resolved in energy and angle. [These were called (e, 2e) experiments.] Deviations from the predictions of the first Born approximation theory were found; this discrepancy may be attributed to long-range Coulomb interactions. In inner-shell studies [called (e, e'-Auger) experiments], the scattered and the Auger electron pair were detected in coincidence. These experiments aimed at the investigation of the generalized alignment tensor of the ion. The major result is that the first-order Born approximation two-step model fails at energies near threshold. Energy shift of the Auger lines of Ar have been observed and ascribed to postcollision interactions – this precludes the interpretation of the results in terms of a pure alignment effect.

A booklet of abstracts or texts of *all* talks given at the Belfast Symposium may be obtained from Dr. Dow-

ker, Department of Physics, Queen's University, Belfast, N-Ireland, BT7 1NN, United Kingdom.

9/1/87

NEWS AND NOTES

Scientific Cooperation Networks in Europe

The European Science Foundation (ESF) has since 1985 launched networks of scientific cooperation. It appears that this framework for this function is now developing into an invigorating mechanism for ESF's role in forging high-quality scientific cooperation in Europe.

A "network" for a specific area is designed to bring together ideas and efforts, human resources and equipment, training capacity, and expertise. Each network is self-managed, in that its organization and scientific supervision is handled by the participating scientists themselves. The networks are very flexible vehicles of communication and cooperation: liaison, contact, information, people-exchange, joint research, and high-level training projects are all possible forms of network operation. In its first phase (the 2 first years of operation), each network is financed by a special Network Seed Fund of the ESF; the amount of support is equivalent to about \$82,000. If the network proves viable, further phases of its operation will be funded by interested member organizations of the ESF or other national or international bodies.

So far, eight networks have been launched, involving 18 ESF countries, and spanning all disciplines. Currently active networks are concerned with the following areas:

- Surface crystallography
- Crystallography of biological macromolecules
- Earth science study centers

- Polar science
- Transport, communications, and mobility
- Molecular neurobiology of mental illness
- History of European expansion.

Observers say that much of the network concept's appeal is rooted in the high degree of scientific independence and self-management, combined with a minimal degree of administrative structure.

I have listings of the coordination committee members of each network, and also short briefing summaries of the seven above-listed networks. I will be glad to share these materials with interested colleagues. Any further information should be asked directly from Dr. Jostein Mykletun, c/o European Science Foundation, 1 quai Lezay-Marnésia, F-6700 Strasbourg, France. Telephone: (011-33) 88-35-50-63.

Paul Roman
2/17/88

Professor Joshua Jortner to Receive 1988 Wolf Prize in Chemistry

Tel Aviv University has announced that Professor Joshua Jortner, incumbent of the Heinemann Chair of Physical Chemistry at Tel Aviv University, will receive the 1988 Wolf Prize in Chemistry, sharing the honor with Professor Raphael D. Levine of the Hebrew University of Jerusalem. The nongovernmental Israeli-based Wolf Foundation gives six international awards annually for out-

standing achievements in Chemistry, Medicine, Mathematics, Agriculture, Physics, and the Arts.

Jortner and Levine were praised by the Chemistry Prize Committee for "their incisive theoretical studies elucidating energy acquisition and disposal in molecular systems and mechanisms for dynamical selectivity and specificity." Their ideas have had an immense impact in many fields of modern chemistry.

"Jortner's ideas and terminology," the Committee added, "became seminal to the study of laser chemistry, multiphoton processes in molecules, relaxation phenomena in condensed phases, and the dynamics of biophysical systems, and had an indelible impact on the modern development of chemical physics and theoretical chemistry."

Jortner, who is President of the Israel Academy of Sciences and Humanities, directs the Zelman Weinberg Physical Chemistry Research Fund at Tel Aviv University. He is the winner of a number of other chemistry awards, including the Israel Prize, the Kolthof Prize given by the Technion-Israel Institute of Technology, the Rothschild Prize, the Weizmann Prize, and the International Academy of Quantum Sciences Award.

The Wolf Prize will be awarded by Israeli President Chaim Herzog in a ceremony to be held at the Knesset in Jerusalem in May. This is the first time that the Wolf Prize in Chemistry has been awarded to an Israeli.

C.J. Fox
3/14/88

A New International Monograph Series in Measurement Science and Technology

John Wiley and Sons Ltd., London, UK, announced the launching of a new book series in Measurement Science and Technology. This irregularly scheduled publication is intended to provide a focus for fundamental, monographic materials in the area of underlying principles involved in measurement system design, application, and appreciation. It is intended that the series will comprise statements of fundamentals, descriptions of current practice, educational course books, and collected keynote papers. It will cover topics such as design, theory of measurement, testing, computerization.

The first volume in the series, scheduled for publication in early 1988, was written by R.V. Jones, FRS, and is titled "Instruments and Experiences". This book consists of republications of selected papers by Professor Jones, introducing each group of papers with a recollection of the circumstances in which the papers were originally produced.

The Chief Editor of the series is Professor P.H. Sydenham, Electronic Engineering, The South Australian Institute of Technology, P.O. Box 1, Ingle Farm, 5098 South Australia.

Paul Roman
9/23/87

European Project on Permanent Magnetic Materials

Historically, many of the fundamental discoveries in magnetism have originated in Europe. However, the amazing decade-old development of extremely powerful permanent ferromagnets, based on rare-earth/iron/boron alloys, was done in the US and Japan. In order to catch up and achieve economic independence in this field, the Commission of the European Communities (CEC) launched a program, called Concerted European Action on Magnets (CEAM). Over 50 laboratories from 11 countries participate, and these institutions have so far received nearly \$3 million CEC support in the form of "stimulation grants." The CEAM links universities, industry, and research institutes.

- The primary aims of CEAM are:
- To develop high-performance iron-based rare-earth permanent magnets
 - To design novel application-devices for these magnets
 - To encourage European cooperation in education of scientists interested in applied magnetism
 - To build an information base and to provide skills permitting European industry to exploit advanced magnetic materials efficiently.

Actually, the research programs fall into three broad areas: materials, magnets, and applications. The materials group is currently working on phase diagrams, searching for new alloys which should have a sufficiently high Curie point and other desirable properties. The magnets group is primarily concerned with the microstructure of magnet alloys and problems of magnet processing, as well as stability. Finally, the applications group focuses on both magnetostatic and electromagnetic applications of the new magnets.

Further information on CEAM should be requested directly from the Commission of the European Communities, Directorate General XII, Rue de la Loi 200, B-1049 Brussels, Belgium. Telephone (011-32-2) 235-7649 or 235-5290.

Paul Roman
9/9/87

New Journal in Nonlinear Phenomena

In February 1988, the UK Institute of Physics in cooperation with the London Mathematical Society, will launch a new quarterly journal, entitled, simply, *Nonlinearity*. The journal is intended to cover everything in this broad area, and will aim at bridging mathematics and physics. It is committed to bring promptly the results of the latest research in nonlinear systems. The journal will not levy page charges. The subscription fee for four issues is set as £110.00 (about \$200.00).

The editors, who say that the journal will have a guaranteed initial circulation of 2500, are calling both for authors and subscribers.

Interested colleagues should contact the Journals Marketing Department, IOP Publishing, Ltd., Techno House, Radcliffe Way, Bristol BS1 6NX, UK.

Paul Roman
12/16/87

The UK Announces National Superconductivity Program

A £16 million (~\$30 million) 3-year national program to keep Britain at the leading edge of superconductivity research has been announced by Lord Young, Secretary of State for Trade and Industry.

This is the first of the national collaborative research programs announced in the UK's Department of Trade and Industry (DTI) White Paper, published on 12 January 1988. It is the result of consultation between the electronics and electrical engineering industries together with the Scientific and Engineering Research Council (SERC) and other government departments. DTI will provide 50 percent of the funds available to the program.

Announcing the program, Lord Young said: "This initiative exemplifies the new DTI approach to research. We want to stimulate companies to work together, pooling their expertise and calling on the best that higher education and European industry can offer. Spreading the costs and benefits of basic research in this way is the best method of encouraging R&D in high risk, precompetitive areas."

Work supported under the program will include research into materials and device applications, as well as research aimed at producing superconductors that work at room temperatures.

Pointing towards applications-oriented work is the DTI's specific welcoming of proposals for industrial collaborative projects in high-temperature superconductivity.

C.J. Fox
3/14/88

Bibliography on Artificial Neural Systems

State-of-the-Art Ltd, a British private company engaged in organizing conferences, seminars, and tutorials in the area of frontier fields of the information sciences, made available a 47-page, up-to-date, alphabetized list of references (books, papers, reports) on artificial neural network systems and their applications. I have a copy and will be glad to share it with qualified colleagues.

Paul Roman
12/20/87

Desert Sand May Be Key To Neutralizing Acid Rain

As announced in a Tel Aviv University release last month, desert sand may help to neutralize acid rain — and Tel Aviv University scientists are determined to find out how and why.

Israel does not suffer from acid rain; on the contrary, rainfall there is often alkaline. Research being carried out at Tel Aviv University indicates that this alkalinity is a result of the incorporation of particles of desert sand into the raindrops.

This finding has emerged from a joint Israeli-West German research project aimed at understanding the processes that create acid and alkaline rain. Germany is eager to solve the problem of acid rain, which is especially acute in the industrial areas of South Germany.

Professor Zev Levin of the Department of Geophysics and Planetary Science, who is also Tel Aviv University's Dean of Research, directs the Israeli side of the project, which is supported by a grant from Israel's National Council for Research and Development and the West German Ministry of Research and Technology. Levin's German counterparts are Professor H.W. Georgii of the Institute for Meteorology and Geophysics at the Johann Wolfgang von Goethe University in Frankfurt, and Dr. W. Jaeschke of the same university.

Levin and his team have developed an original research method which involves looking very closely at the makeup and behavior of raindrops, and at the cloud

droplets out of which raindrops form. They spend much of their time measuring the size of cloud drops and raindrops and analyzing their chemical content as a way to understand how the cloud droplets were formed and what happens to them during their various growth stages.

"We have discovered," Levin said, "that, on occasion, rain in Israel can be very alkaline. This usually occurs after dust storms, so we can conclude that alkaline rain is the direct result of the incorporation of dust particles from the desert into the raindrops."

"Our measurements show that the cloud droplets, during their initial growth stages, and before the raindrops are formed, are somewhat acidic. During this time, the dust particles are not incorporated into the drops, but are found between them. These particles are later captured by the falling raindrops and change the acidity of the rain to an alkaline state."

The team has also developed techniques for identifying the chemical content of the drops and making quantitative estimates of amounts of various pollutants, such as sulfates. Various numerical models which simulate the development of rain in the atmosphere have also been devised, as well as a very detailed model of the development of raindrop distribution below the cloud base.

On the German side, research focuses on the acidity of fog in forested areas, and how this affects vegetation.

By understanding how acid rain is formed, the scientists hope to be able to pinpoint its causes, and with this informa-

tion in hand, begin to search for a preventive.

The results of the project have been discussed at a German-Israeli workshop held in Israel, and will be presented at the International Cloud Physics Conference to be held in West Germany next summer.

C.J. Fox
3/14/88

Information Exchange for Artificial Neural Systems

An informal information exchange center for neural network systems, neurocomputers, and related areas has been set up which will gather and disseminate timely information on principles, theory, logic, organization and structure, systems-theoretical aspects, technology, and applications for these systems. It will also inform participants of forthcoming meetings, and provide up-to-date lists of participants. Participants are requested to submit preprints, reprints, references, conference calls, private communications, opinions; they may also ask specific questions. Participation is open for all interested and qualified scientists.

The contact address is: Dr. Jörg Becker, ET/Physik, Universität der Bundeswehr (München), D-8014 Neubiberg, West Germany. The telephone number is: (011-49-89) 6004-2284 or 6004-4036.

Paul Roman
2/17/88

ONRL REPORTS, SCIENCE NEWSBRIEFS, AND MAS BULLETINS

Reports

To request reports, indicate the report number (in parentheses after the title and author's name) on the self-addressed mailer (the back cover) and return it to ONR, London.

Biological Sciences

Fourth European Conference on Biotechnology, by Claire E. Zomzely-

Neurath. (8-001-C) Presentations in selected topics given at this meeting, held in June 1987, are summarized. Based on the variety and depth of the presentations at this conference as compared to those at the conference in previous years, the author states that biotechnology research in Europe has expended tremendously and that European scientists are in the forefront of research in biotechnology.

Biotechnology Congress: BIOTECH-NICA '87 Hannover, by Claire E. Zomzely-Neurath. (8-002-C) This is a summary of the third international exhibition and congress for biotechnology, held in September 1987 at Hannover, West Germany. Topics of the presentations reviewed are polypeptides in therapy, enzymatic and microbial transformation, and fundamentals of bioprocess engineering.

International Conference on Separation of Biotechnology: Reading, UK, by Claire E. Zomzely-Neurath. (8-003-C) Selected presentations given at this conference, held in September 1987, are reviewed. Topics are: cell harvesting and disruption, adsorption and chromatography, analytic techniques and process control, liquid-liquid extraction, and membrane extraction.

Material Sciences

Nitrogen Ceramics Meeting in France, by Louis Cartz. (8-004-C) Presentations given at this meeting—EN17—held in Rennes, France, in September 1987, are briefly reported. A very wide range of nitrogen ceramics properties was discussed at the meeting, in particular, their chemistry, crystallography, and sintering behavior.

Ocean Sciences

Assessment of Ocean Optics, Remote Sensing and Numerical Modeling in Europe—1986-87, by Jerome Williams. (8-005-R) The focus of this report is on

those institutions which were doing the most significant work in Europe in optical oceanography, remote sensing, and numerical modeling during 1986-87. The work of each of the institutions in its strong area of research is reviewed.

Science Newsbriefs

The following issues of *Science Newsbriefs* have been published to date during 1988. *Science Newsbriefs* provide concise accounts of scientific research developments, meeting announcements, and science policy in Europe and the Middle East. Please request copies, by number, from ONR, London.

- 6-1 Composite Materials Meetings in Europe 1988, by Louis Cartz
- 6-2 Materials Meeting in Europe 1988, by Louis Cartz
- 6-3 Atomic Scale Microscopy at Oxford, UK, by Louis Cartz
- 6-4 BEM 10-Boundary Element Conference, by David Feit

MAS Bulletins

The following *Military Applications Summary (MAS) Bulletins* were published during March and April. The *MAS Bulletin* is an account of accomplishments in European naval research, development, test, and evaluation. Request copies of the Bulletins, by number, from ONR, London.

- 21-88 Mandarin Passive Acoustic Operator Training System
- 22-88 Near Surface Current Measurements Using A Satellite Telemetering Buoy
- 23-88 Hydrocyclone Oil/Water Separations
- 24-88 New Towed Body Depressor Design
- 25-88 Excaliber 180
- 26-88 A New European Venture in Integrated Optics
- 27-88 First Quarterly Index 1988

REPORTS ON EUROPEAN SCIENCE AND TECHNOLOGY FROM OTHER COMMANDS

Reports

Information on each of the reports listed below was furnished by the activity identified by the abbreviations for that office. Requests for copies of or information about the document should be addressed to the appropriate office:

USARDSG—US Army Research Development and Standardization Group, Box 15/65, FPO New York, 09510-1500

EOARD—European Office of Aerospace Research and Development, Box 14, FPO, New York 09510

Aerospace

The Sowerby Research Center of British Aerospace, by LTC Bob Winn, EOARD. (5 pp) [EOARD-87-108]

The Sowerby Research Center is the focal point for all basic research conducted by British Aerospace. This report describes the Center and discusses the research currently underway in each of the six departments. The departments are Information Technology, Aerodynamics and Vulnerability Research, Computational Physics and Special Studies, Human Factors, Laser Systems, and Materials Branch.

The JAS 39 Gripen Aircraft, by MAJ Tom Speer, EOARD. (8 pp) [EOARD-87-103]

The JAS 39, known as the Gripen, is a new multi-role fighter aircraft being built in Sweden by SAAB. The JAS 39 is designed to offer a low life cycle cost; perform fighter, attack, and reconnaissance roles; and operate from dispersed bases. This report is based on briefings given by SAAB in October 1987, and presents a

technical overview of the JAS 39 configuration and technologies. It describes the design considerations behind the operational concepts, flight control system, cockpit, avionics, aerodynamics, weapons, and other subsystems.

Biological Sciences

Oral and Dermal Sustained Release Technology Postgraduate School of Studies in Pharmacy at the University of Bradford, UK, by MAJ Jim McDougal, EOARD. (7 pp) [EOARD-LR-87-90]

A visit to the laboratory of Professor Brian Barry provided an overview of some exciting and state-of-the-art developments in pharmaceutical formulation and skin penetration technology. His drug delivery group has researched, developed, and is in the process of patenting a technology for sustained release of drugs called Optimised Sustained Action Tech-

nology (OSAT). OSAT combines innovative theories with modern materials to produce multiparticulate oral dosage forms with controlled, differential scanning calorimetry (DSC) to investigate the mechanism of action of chemicals known to enhance penetration of drugs through the skin. They use DSC to examine the thermal behavior of human stratum corneum, and whether accelerants such as Azone and dimethylsulfoxide enhance penetration by modifying this behavior.

Visual Evoked Responses, Movement Perception, Image Processing and Binocular Contrast Detection, by MAJ Jim McDougal, EOARD. (5 pp) [EOARD-LR-87-89]

A visit with Professor David Pickwell and his scientists provided an overview of some interesting studies of the human visual system. Visual evoked responses to a suprathreshold stimulus (reversing checkerboard pattern) are being thoroughly assessed as a means of quantitating visual acuity using an extrapolation technique. The effects of adapting velocity, luminance, temporal frequency, and optical image degradation on detection of oscillatory movement are being investigated. Digital image processing of ocular photographs is being investigated to facilitate the quantitation of optical lesions. Preliminary studies on analysis of diabetic retinopathy increased accuracy for detection of subtle changes. Binocular contrast detection with unequal monocular luminances is being investigated to examine summation mechanisms and predict binocular performance from monocular sensitivity.

Computer Sciences

Knowledge-Based Information Systems Symposium - 1987, by LTC Bob Winn, EOARD. (8 pp) [EOARD-LR-87-104]

The SHAPE Technical Center in the Netherlands hosted a 3-day conference titled "Symposium on Knowledge-Based Information Systems for Military and C³I Applications - 1987" on 20-22 October 1987. The overall objective of the symposium was to assess the current state of the art in knowledge-based information systems and to determine if there are current applications of the technology which could be of use to SHAPE and NATO. This report consists of a brief overview of the conference. The symposium program is attached to the report to give the title, author and organization for each paper.

Electronics

Millimeter Wave Device Research at the Technical University of Munich, by MAJ Mel Townsend. (21 pp) [EOARD-LR-87-105]

A strong research effort in MMW and microwave devices technology is underway at the Technical University of Munich. Two TUM research institutes are working with planar and hybrid microwave and MMW circuits, both gallium arsenide and silicon substrate based. A strong expertise exists in the design of high-power impatt diodes (both the devices and the packaging). TUM is also involved with MMIC technology, and is working on microwave circuits on ceramic and silicon substrates. This report describes research in more detail and includes university literature and reprints.

Fluid Mechanics

Fluid Mechanics Meetings in Europe, 1988-1990, by MAJ Tom Speer, EOARD. (9 pp) [EOARD-LR-88-01]

This report consists of a comprehensive list of conferences and short courses related to fluid mechanics, giving dates, location, subject, and address of person to contact.

Acoustical Fluid Control, by MAJ Tom Speer, EOARD. (6 pp) [EOARD-LR-88-07]

Developments at the Cambridge University Engineering Department have shown the potential to control a wide range of fluid phenomena using sound waves. Demonstrated applications include the active control of compressor stall, stabilization of combustion instabilities, suppression of wing flutter, and the cancellation of noise propagation using anti-noise. The control of compressor stall demonstrated the ability to operate well above the surge line for the uncontrolled system. Stabilization of afterburner rumble has been shown to be feasible by stabilizing the combustion in a Rijke tube, and through larger scale experiments. Structural control using wave propagation concepts are also demonstrated.

Material Sciences

Rapid Solidification Processing, by LTC Jim Hansen, EOARD. (7 pp) [EOARD-LR-87-107]

Dr. Howard Jones leads an effort to develop aerospace metal alloys (aluminum and magnesium) and intermetallics using rapid solidification processing. Iron aluminides are melt

spun into ribbons and tested for hardness and ductility. Magnesium RSP splats (alloyed with Al, Zn, and/or Mn) are being consolidated and processed by extrusion.

Inflatable Rigidized Structures for Space, by LTC Jim Hansen, EOARD. (4 pp) [EOARD-LR-88-08]

Large space structures made of Kevlar/epoxy composite material are being developed at Contraves AG in Zurich, Switzerland. Deployment involves pressurization and thermal cure. A 3-m scale antenna has been built and tested. Actual antenna systems are planned to 20 m. The deployment system is applicable to other large space structures.

Physics

Resonant Tunneling Studies, by Dr. Eirug Davies, EOARD. (2 pp) [EOARD-LR-87-100]

Nottingham University, England, is one of the participants in the UK initiative on Low Dimensional Structures. The Physics Department specializes in resonant tunneling phenomena and possess a molecular beam epitaxial reactor for growth within the GaAlAs system. Interesting sequential tunneling effects have recently been identified.

High-Power CO₂ Industrial Laser Systems, by Dr. Stacey Lazdinis, EOARD. (4 pp) [EOARD-LR-87-98]

The Laser Applications Group at Culham Laboratories has done significant work in developing high-power CO₂ industrial laser systems. Currently it is playing a major role in the multinational European BRITE Program and is the UK lead on the EUREKA Excimer effort. The work of Dr. Harvey Rutt, the working leader of the Group, is reviewed.

First International Laser M2P Conference, by Dr. Stacey Lazdinis, EOARD. (5 pp) [EOARD-LR-87-99]

The proceedings of the First International Laser M2P Conference, which was held in Lyon, France, between 7 and 9 July 1987, are summarized. Presentations dealing with ultrafast phenomena, high-resolution spectroscopy, deterministic chaos in laser systems, metal cluster spectroscopy, laser-induced fluorescence, short wavelength chemical lasers, anti-Stokes Raman laser studies in the UV and VUV, excimer lasers, high-accuracy laser diagnostics of discharges, intracavity absorption spectroscopy, and nonlinear Raman spectroscopy are summarized.

The Gas Laser Research Group, by Dr. Stacey Lazdinis, EOARD. (3 pp) [EOARD-LR-87-101]

This report summarizes the work of Dr. Colin Webb in rare gas halide (RGH) and metal vapor lasers. Dr. Webb is head of the Gas Laser Research Group at Oxford University's Clarendon Laboratory and Chairman of Oxford Lasers, Ltd. in the UK. Specifically, the research performed by him and his colleagues in copper-vapor and gold-vapor lasers; cryogenic gas purification; four-wave-mixing; and Excimer laser discharge technology is described.

Semiconductor Physics at the University of Innsbruck, by LTC LaRell Smith, EOARD. (10 pp) [EOARD-LR-88-04]

The Experimental Physics Institute at the University of Innsbruck is one of the best and most prolific in Europe in the field of semiconductor physics. They have recently been doing work on narrowband photodetectors which are produced by combining MIS structures with a surface grating. These have been shown to have 20-30 percent quantum efficiency and very narrow detection bands which, through appropriate structure changes, can be tuned over a wide range of the visible and UV spectrum. This report describes that work as well as work on stimulated emission from p-germanium in crossed fields.

Non-Linear Optical Materials Work at Heriot-Watt University, by LTC LaRell Smith, EOARD. (7 pp) [EOARD-LR-88-03]

The physics department at Heriot-Watt has been one of the world leaders in nonlinear optics and optical bistability for many years. Much of their work has been directed at demonstrating the feasibility of optical computing. They

are now significantly expanding their efforts in the materials area to investigate the fundamentals of structure- and materials-related questions relating to nonlinear materials. This report summarizes some of the recent work in nonlinear optics and describes the new materials work which will be undertaken in collaboration with the OCLI (Optical Coatings Ltd., Incorporated) firm in Dunfermline, Scotland.

Laser Chemical Processing and Diagnostics, by Dr. Stacey Lazdinis, EOARD. (4 pp) [EOARD-LR-88-22]

The research of Professor Dieter Bauerle of the Applied Physics Department of the Johannes Kepler University at Linz, Austria, in laser chemical processing and diagnostics is described. Specifically, his research in laser-induced chemical vapor deposition (LCVD); gas phase Raman diagnostics of chemical vapor deposition (CVD) systems; and laser-induced chemical etching and reduction of materials having applications in microelectronics is reviewed and summarized.

VULCAN and SPRITE: Europe's Most Powerful Lasers, by Dr. Stacey Lazdinis, EOARD. (4 pp) [EOARD-LR-88-21]

Europe's most powerful laser, VULCAN, and the world's most powerful laser dedicated to research, SPRITE, both located at the Central Laser Facility (CLF) of the UK's Rutherford Appleton Laboratory are described in detail (VULCAN is a high-power Nd:Glass laser radiating at 1.053 μ m, while SPRITE is an electron beam pumped KrF excimer laser system radiating at 249 nm.) The research performed during the past year with both devices in the fields of ultradense plasmas, x-ray generation,

and x-ray laser radiation production are briefly summarized.

Electromagnetic Launch Technology Applications Conference, by Dr. Vince Donlan, EOARD. (4 pp) [EOARD-LR-88-02]

The fourth Executive Seminar on Electromagnetic (EM) launcher applications was held in London, England on 18-19 November 1987. This meeting was jointly sponsored by the Defense Advanced Research Projects by the Defense Advanced Research Initiative Agency (DARPA) and the Strategic Defense Initiative Office (SDIO). The current status of EM launcher technology was reviewed and details of current strategic and tactical applications of EM guns were presented. This report summarized the technical contents of this 2-day meeting.

Science Education

Institutions of Higher Education in Dublin, Ireland, by COL Phil Conran, EOARD. (4 pp) [EOARD-LR-88-16]

This trip report is a summary of my impressions of the facilities and capabilities of the institutions of higher learning located in Dublin, Ireland. The five institutes I visited offer different degrees of scientific expertise, some of which might be of interest to US agencies seeking superior research facilities and personnel.

ONRL COSPONSORED CONFERENCES

ONR, London, can nominate two DOD employees for registration-free participants in the conferences ONRL supports. Readers who are DOD employees and are interested in a free registration to one of these conferences should write to the Scientific Director,

ONRL, Box 39, FPO New York 09510. (Please site reference number.)

Second Conference on Hyperbolic Problems, Aachen, West Germany, March 1988. (81009)

Structure and Function of the Cytoskeleton, Lyon, France, April 1988. (81005)

Modulation of Short Wind Waves in the Gravity-Capillary Range by Non-uniform Currents, Gergenaan-Zee, the Netherlands, 3-5 May 1988. (81006)

A Critical Analysis of Synthetic Aperture Radar, Capri, Italy, 14-16 May 1988. (81014)

Critical Currents in High Tc Super Conductors, Birmingham, UK, 16 May 1988. (81021)

Spring School on Surface and Technology, Ankara, Turkey, May 1988. (81024)

11th European Conference on Thermophysical Properties, Umea, Sweden, 13-16 June 1988. (810017)

Conference on Mathematical Methods in Computer Aided Geometric Design, Oslo, Norway, 16-22 June 1988. (810019)

Symposium Ontogen of Neural Peptides, Jerusalem, Israel, 19-24 June 1988. (81007)

Dynamics of Protein Development and Function, Heidelberg, West Germany, 26 June-1 July 1988. (81008)

3rd Annual Conference on Operator Theory and Operator Algebras, Cork, Ireland, 29 June-2 July 1988. (810016)

Symposium on Application of Laser Anemometry to Fluid Mechanics, Lisbon, Portugal, 11-14 July 1988. (81009)

Nonlinear Problems and Symmetries, Schloss Hofen, Austria, 25-29 July 1988. (81010)

Solid Compounds of Transition Materials, Oxford, UK, 4-8 July 1988. (81011)

Thermodynamics Applied to Biological Systems, Sta Margherita, Italy, 11-17 September 1988. (81012)

Physical Mechanisms in Polymer Failure, Lausanne, Switzerland, 16-30 September 1988. (810023)

Technical Development in the Area of Submillimeter and Far Infrared Technology, Zermatt, Switzerland, 22-25 September 1988. (81022)

2nd Workshop on Imagery and Cognition, Padova, Italy, 21-23 September 1988. (810018)

Spring School on Surface and Technology, Ankara, Turkey, May 1988. (810024)

TECHNOLOGY ROUNDUP-ITALY

The items below were received from the American Embassy in Rome. For further information, contact Dr. Gerald Whitman, Office of the Science Counselor, American Embassy, Rome, APO New York 09794-0007.

Ansaldo Develops Superconducting Motor. The Genoa-based company Ansaldo is developing a superconducting electric motor, the first of its kind in Italy. The motor, based on the same principles as the one recently developed at Argonne National Laboratory, will be ready for testing this spring.

New Composite Material Tested at Montedison. Sheets made of polyethylene terephthalate reinforced with long glass fibers are being tested at the Guido Donegani Research Center of the chemical company, Montedison. This composite material has high thermal resistance (up to 240C) as well as high resistance to shock and tear. The sheets can be stamped like ordinary metal sheets and are being explored for use in the automobile industry.

Biomedical Institute Established in Bari. The University of Bari is founding an international biomedical institute to be located near Brindisi. The institute will focus research on: (1) identification and mechanisms of macromolecules influencing cellular growth, differentiation, transformation and defense; (2) biomembranes; (3) activities of molecules of pharmacological interest.

Cell Proliferation Protein Discovered in Milan. Researchers in Milan have isolated a protein considered to be responsible for the abnormal proliferation

of cells, causing tumors of the hypophysis. The protein acts on cyclic adenosine monophosphate (CAMP), one of the factors regulating cell proliferation, producing abnormal CAMP activity and continuous cell proliferation. This "Q" class protein has been isolated only in hypophysis tumors, but the researchers do not exclude its presence in other tumors.

Natural Substance Acts as Cerebral Antidepressant. Professor Erminio Costa recently identified a peptide in mammal brains that links up with the same receptors that are bound by traditional antidepressant drugs called diazepam binding inhibitor (DBI). Researchers hope the peptide will lead to new types of natural antidepressants, thereby avoiding the use of substances considered to be alien to complex cerebral chemistry.

Laser Drill for Dentistry. Professor Leonardo Masotti of the Institute of Applied Electronics of the University of Florence has developed a laser beam dentist's drill which will be tested on an experimental basis in Italy. The Office of Health Programming of the Ministry of Health is consigning 12 of the new instruments to the Tuscany, Emilia, and Lombardy regions for testing in the University of Pisa, Bologna, Milan, and Ferrara as well as in private dentists' laboratories in Florence and Siena under a 6-month evaluation program. The instrument uses two lasers; the first (carbon dioxide) employs a 10.6-micron beam to disintegrate caries; the second (neon and helium) is used to illuminate the area where the principal beam is directed.

Erbamont Builds "Research City." Erbamont, a company of the Montedison Group, is building at Nerviano (near Milan) a research city which will focus on pharmaceuticals and biotechnology. When completed in 1990, the center will employ 1000 researchers working to develop new drugs for oncology, cardiovascular diseases, immunology, anti-infective drugs, and drugs for the central nervous system. In 1988, Erbamont will spend 200 billion lire (about \$164 million) for research.

National Campaign to Measure Acid Rain. The National Research Council's Institute for Atmospheric Pollution, together with the Ecological Research Group (GRE), and the Italian Society for the Progress of Sciences (SIPS), are launching a national campaign for the measurement of acid rain. Approximately 100,000 volunteers recruited from schools and environmental groups will collect samples in 160 areas of 150 square kilometers. The data will be collected and centrally computerized. The first campaign will last from January 13 through February 21 and the second one will occur in the springtime.

Urban Waste Fuels Cement Plant. Technicians of the National Research Council, ENEA, and Enichem have created a fuel from urban waste composed of paper, plastics, and wood fibers. Known as RDF, the material is employed in a Ravenna cement plant as fuel, allowing a 15-percent saving in coal and a 30-percent decrease in urban waste volume. In addition, the ashes obtained are used as an additive for the cement.

OVERSEAS TRAVELERS

Notes on trip reports to locations in Europe and the Middle East which have been received by ONRL are reported below. For details, contact the traveler directly.

Oceanography

Traveler: Paul Scully-Power, Research and Technology Staff, Naval Underwater Systems Center, New London,

Connecticut 06320. Scully-Power, the first scientist to observe and record ocean phenomenon as one of the crew of a space shuttle flight, visited the Department of Applied Mathematics and Theoretical Physics at the University of Cambridge at the invitation of Dr. Michael McIntire. While there, Scully-Power gave a standing-room-only lecture entitled "Oceanography from Space, Spiral Eddies, and

Ocean Nonlinear Dynamics." The lecture generated considerable interest and resulted in discussions in depth with Professor Michael Longuet-Higgins and Drs. Paul Linden and Peter Haynes. There was much to discuss: Scully-Power says that the dynamics of ocean spiral eddies are as yet unknown, and have raised many technical issues in the ocean research community.

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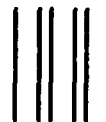
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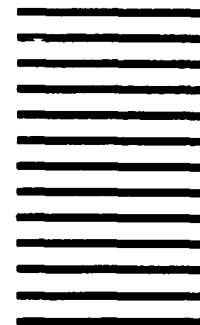
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